

# **Semi-Microscopic and Phenomenological Studies of Nuclear Effective Interaction**

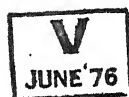
A Thesis Submitted  
In Partial Fulfilment of the Requirements  
for the Degree of  
**DOCTOR OF PHILOSOPHY**

By  
**MAHESH PRAKASH**

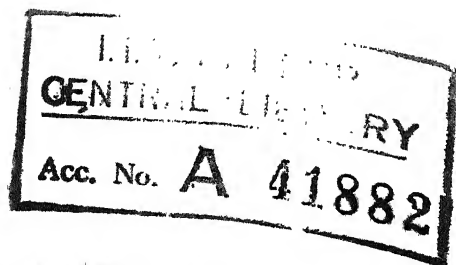
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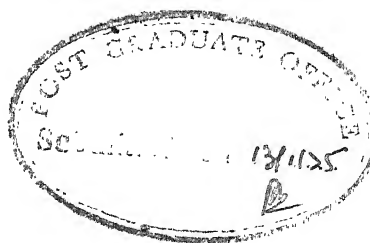
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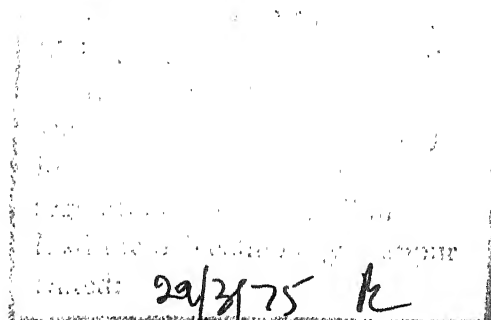
# CERTIFICATE

Certified that the work presented in the thesis entitled "Semi-Microscopic and Phenomenological Studies of Nuclear Effective Interaction" is the original work of Mr. Mahesh Prakash carried out under my supervision.

This work has not been submitted anywhere else for a degree.

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## SYNOPSIS

In the present work, we have studied low-lying energy levels of light and intermediate nuclei ( $6 \leq A \leq 92$ ) with realistic as well as phenomenological interactions. The thesis consists mainly of four chapters. First chapter gives a review of recent developments in nuclear theory, particularly the structure aspect. In Chapter II we first present a review of conclusions as arrived at by different researchers who have made microscopic calculations of renormalization corrections to free N-N interaction. Purely microscopic approach turning out a failure, they suggest the introduction of phenomenological and/or experimental information into microscopic calculations. Taking this clue, we start with Sussex matrix elements (SME) as effective interaction in first order. Under the assumption that the potential which the SME represent is momentum independent and is a combination of central, spin-orbit and tensor parts, we first calculate the spectra of  ${}^6\text{Li}$ ,  ${}^{18}\text{F}$ ,  ${}^{18}\text{O}$ ,  ${}^{42}\text{Sc}$ ,  ${}^{42}\text{Ca}$ ,  ${}^{58}\text{Ni}$  and  ${}^{92}\text{Zr}$  nuclei with each of these components and with the combinations central + spin - orbit, central + tensor, and also with the total SME. We conclude that the spin-orbit part is almost ineffective for two-body spectra. However, the tensor part is more important, particularly for  $T = 0$  states, and finer details of the spectra are dependent

on presence or otherwise of the tensor part in the interaction although the central part is the most important and dominant contributor to level energies. The calculated level energies are not in agreement with experimental values. The off-diagonal tensor force  ${}^3S_1 - {}^3D_1$  only effectively renormalizes the triplet central interaction, the  $T = 0$  low-lying states are predominantly  ${}^3S_1$  relative states and the experimental values of matrix elements therein also bear the maximum uncertainties. We find that few of the low-lying  $T = 0$  levels of  ${}^6\text{Li}$ ,  ${}^{18}\text{F}$  and  ${}^{42}\text{Sc}$  nuclei can be reproduced if the  ${}^3S_1$  relative matrix elements are multiplied by a suitable factor  $(1 + \alpha)$ , i.e., all the renormalization corrections to the  $T = 0$  SME can be effectively simulated by  $\alpha$  times the bare interaction matrix elements in  ${}^3S_1$  relative states. The calculated ground state  $0^+$ ,  $T = 1$  level in  ${}^{18}\text{O}$ ,  ${}^{42}\text{Ca}$ ,  ${}^{58}\text{Ni}$  and  ${}^{92}\text{Zr}$  nuclei turns out to be above the experimental position. Addition of a constant strength pairing force is shown to reproduce the correct ground state energy with an appropriate choice of the strength. An improvement over this is the addition of a  $\delta$ -function force (instead of the pairing force) which besides reproducing correct ground state energy, also improves some of the higher levels. Further addition of a quadrupole force of suitable strength is found to simulate the renormalization of the long range part as needed for higher levels. In

general, J-dependent effective interactions can be established, for both  $T = 0$  and  $T = 1$  levels, through introduction of phenomenology. In Chapter III, the problems of  $^{40}\text{K}$  and  $^{38}\text{Cl}$  nuclei are investigated with phenomenological effective interactions of Gaussian radial shape and containing central, spin-orbit and tensor dependences. The forms of effective potential tried are central, central + spin - orbit, central + tensor and central + spin-orbit + tensor. The parameters are deduced by making a  $\chi^2$  fit to experimental level energies of  $^{40}\text{K}$ . Validity of the parameters is checked by applying them to energy level calculation for the  $^{38}\text{Cl}$  nucleus. The lowest  $3^-$  state is not correctly described in both  $^{40}\text{K}$  and  $^{38}\text{Cl}$  nuclei. Except for this, the predicted energy levels in  $^{38}\text{Cl}$  are in good agreement with experimental energies. In Chapter IV, we make a general study of the two-nucleon interaction. We assume a Yukawa shaped central force of arbitrary strength and range parameters and calculate the effect of configuration mixing on  $T=0$  and  $T=1$  levels of  $(0f_{7/2})^2$  configuration in  $^{42}\text{Sc}$  as the space dimensionality is increased by adding configuration-after-configuration. Within fp-shell we calculate the splitting between centroids of  $T = 1$  and  $T = 0$  levels of the  $(0f_{7/2})^2$  configuration as a function of the various  $A_{TS}$  strength parameters and the space dimensionality. / For a randomly chosen set of parameters,

we find that the levels under consideration do not approach a saturated energy value as the space is expanded and sometimes the inclusion of  $0f_{5/2}$  configuration is found to have larger effect than that of few of the other low-lying configurations. This puts suspicion over effective interaction derived within fp-shell since it appears that the single particle energy of an orbit is not the only decisive factor in determining its effect on low-lying energy levels and it might not be an honest attempt to parametrize an effective interaction wherein the effects of the more-important-than-the-truncated-model-space-configurations are absorbed by a forcible fitting of parameters. We justify it by approximately calculating the configuration mixing contributions to  $0^+$  and  $1^+(0f_{7/2})^2$  configuration levels, of all configurations lying up to  $0i_{13/2}$  single particle level.



## CHAPTER I

### INTRODUCTION

#### I.1 DEVELOPMENT OF FORMALISM FOR NUCLEAR STRUCTURE CALCULATIONS:

Understanding the structure of finite nuclei requires the understanding of the basic nucleon-nucleon (N-N) force. The nuclear forces between two nucleons are believed to be mediated by exchange of mesons which, hence, involve finite time for interaction to take place. The first assumption that is made is that even though the interaction might be meson-mediated but we assume it to be instantaneous i.e. we assume potential interactions. Then, the many-body Hamiltonian for a system of A particles is obtained as the sum of individual kinetic energies and sum of all interactions

$$H = T + V \quad (1.1)$$

$$\text{where } T = \sum_{i=1}^A T_i \quad (1.2)$$

One, then, solves the many-body Schrodinger equation

$$H \Psi = E \Psi \quad (1.3)$$

for the system's total energy  $E$  corresponding to the  $A$ -particle wave function

$$\Psi = \Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_A) \quad (1.4)$$

In principle, the problem is solved if we know the mathematical form of  $V$  and the method of exactly solving the many-body Schrodinger equation. Since none of these is available, we have to resort to approximate methods. We postulate models which might in some way reduce troubles.

In view of strong interactions, liquid drop model was the first to be proposed which satisfactorily explained the bulk properties of nuclei e.g. binding energies. One important conclusion that was derived on this model was that for most part of it the nuclear interaction is two-body in character i.e. the total potential energy can be written as

$$V = \sum_{i < j}^A V_{ij} \quad (1.5)$$

However, the existence of magic numbers demanded a model wherein the nucleons might be considered as moving

almost independently of each other so as to retain their individuality in order to be able to fill quantized orbits. Thus came the independent particle model (IPM) with infinite harmonic oscillator well and a one-body spin-orbit potential constituting the average field. However, this model could not successfully account for magnetic moments and failed completely in describing excited states, particularly in case of nuclei which have more than one particle in last partially filled orbit. It was, therefore, assumed that the two-nucleon interaction is not completely exhausted in giving rise to the average potential and a part of it, the residual interaction, still operates between valence nucleons. The IMP with residual interactions was called 'the shell model'. Thus, the Hamiltonian (1.1) can be rewritten as

$$\begin{aligned} H &= T + U + (V - U) \\ &= H_0 + H' \end{aligned} \quad (1.6)$$

where  $U$  is the average potential,

$$H_0 = T + U \quad (1.7)$$

is the sum of single particle Hamiltonians and

$$H' = V - U \quad (1.8)$$

is the residual interaction.

Under the assumption of weak interactions, the many-nucleon wave function (1.4) can be written as product of wave functions for individual particles

$$\Psi = \Psi_1(\vec{r}_1) \Psi_2(\vec{r}_2) \dots \Psi_A(\vec{r}_A) \quad (1.9)$$

Dividing the problem into a core part and the valence nucleons part, the wave function (1.9) can be regrouped as

$$\Psi = \Psi_c \Psi_v \quad (1.10)$$

where  $\Psi_v$  is the product of single particle wave functions of  $v$  valence nucleons and  $\Psi_c$  is the wave function for  $(A-v)$  core nucleons. Then, the total energy  $E$  can be written as a sum of core and valence nucleons' energies, the interaction between valence nucleons and core being included in the energy of valence nucleons. If the core is not disturbed while considering different levels and one is interested in splittings of energy levels rather than the absolute level energies, the core energy simply drops out. Thus, finally, the equation to be solved is

$$(H_0 + V)\Psi = E\Psi \quad (1.11)$$

where the variables pertain to valence nucleons only and the subscript  $v$  will not be put henceforth. We have also slightly changed the notation in that now  $V$  denotes the residual interaction between the valence nucleons (instead of  $H'$  as earlier).

Starting with the lowest partially filled orbit, the unperturbed (i.e. no residual interactions) wave functions  $\phi_i$  span an infinite dimensional Hilbert space such that

$$H_0 \phi_i = \epsilon_i \phi_i \quad i = 1, 2, \dots \infty \quad (1.12)$$

where  $\epsilon_i$  is the sum of single particle energies of valence nucleons in the configuration  $\phi_i$ . The problem, thus, finally reduces to that of understanding the potential  $V$  such that eq. (1.11) when solved with  $V$  gives eigenvalues  $E$  which are in agreement with experimental level energies and wave functions  $\Psi$ 's which also properly describe other nuclear properties e.g. electromagnetic transition rates etc.

While in a stationary orbit, the nucleons, as a result of residual interaction, can undergo virtual excitations for time limits as prescribed by uncertainty principle. These virtual excitations, although experimentally undetectable, do affect the energies. If the virtual

excitations are considered, the wave functions for valence nucleons can no longer be taken as pure  $\phi_i$ 's. Also, beforehand there is no way of knowing how many orbits are mixed. Hence, the wave function, in presence of residual interactions, has to be written as

$$\Psi = \sum_{i=1}^{\infty} a_i \phi_i \quad (1.13)$$

The eq. (1.11) is then equivalently written as

$$\sum_i^{\infty} a_i (\epsilon_i \delta_{ij} + \langle \phi_j | V | \phi_i \rangle) = E a_j \quad (1.14)$$

$$j = 1, 2, \dots, \infty$$

Solving the set of infinite number of equations (1.14) is equivalent to diagonalizing the matrix of  $(H_0 + V)$  in the infinite dimensional Hilbert space spanned by the basis vectors  $\phi_i$ . If  $V$  is very weak, one could try to solve the problem by retaining only a finite number of terms in the expansion (1.13). However, such hope fails to materialize if  $V$  induces strong short range correlations. In presence of strong repulsions, the nucleons can scatter into any orbit and any number of times. It would be of no use finding some way of diagonalizing infinite dimensional matrices since the perturbation theory would not be applicable for calculating matrix elements of  $V$ .

In presence of singularities in  $V$ , one uses reaction matrix derived from  $V$ , instead of using  $V$  directly,

$$G(E) = V + V \frac{Q}{E - H_0} G(E) \quad (1.15)$$

where  $G(E)$  is the reaction matrix operator,  $Q$  is the Pauli operator allowing interacting particles to scatter into unoccupied states only and  $H_0$  is the unperturbed Hamiltonian acting in the space of intermediate states.

Once the two-nucleon potential is chosen - it may be a smooth phenomenological potential or a reaction matrix derived from free N-N interaction containing hard core, the next step is to solve the self-consistent Hartree-Fock (HF) problem for single particle energies and wave functions which are then used in solving eq. (1.11) with the potential  $V$  between valence nucleons same as the original two-nucleon potential. Such attempts<sup>1</sup> have shown that the results calculated with HF single particle wave-functions are similar to those obtained with harmonic oscillator wave functions. Thus, instead of solving the self-consistency problem, one generally assumes the single particle orbitals as pure harmonic oscillator wave functions and takes single particle energies from

experimental spectra of neighbouring odd-mass, one-valence-nucleon nuclei.

If  $V$  contains singularities, we can avoid them in diagonalization by introducing reaction matrix in eq. (1.14) but, then,  $G$  has to be calculated first using eq. (1.15) where one again faces  $V$ .

A method, called the separation method, to handle the singularities in  $V$ , was developed by Moszkowski and Scott<sup>2</sup>. In this method, the total potential  $V$  is divided into a short range part  $V_S$ , which contains all singularities and a long range part  $V_L$ , which is smooth and weak, such that when two nucleons interact,  $V_S$  itself does not produce any phase shift i.e. if the two interacting nucleons do not come close enough so that  $V_S$  be felt, the presence of  $V_S$  is as good as its absence. Thus, the residual interaction is effectively just the long range part  $V_L$ . Yet another method of handling singularities is the unitary-model-operator approach of Shakin et.al.<sup>3</sup> where one does not calculate reaction matrix. Instead, they introduce correlated wave functions which vanish whenever two nucleons come closer than hard core radius.

The calculation of matrix elements of a hard core interaction becomes a two-step process: one has to first



construct the potential and then derive the reaction matrix. Experimentally, all information about the N-N interaction is contained in the phase shifts and, in principle, it should be possible to relate the matrix elements of the interaction to the measured phase shifts, thus skipping the intermediate step of constructing a potential. Such an approach has successfully been attempted by Elliot et.al.<sup>4</sup> employing auxiliary potential method. The matrix elements obtained are generally called Sussex matrix elements (SME). The analogy of this method to Moszkowski-Scott separation method for deriving reaction matrix elements from phase shifts has also been established<sup>5</sup>. Sanderson et.al.<sup>6</sup> have also suggested a way of incorporating short range repulsion in the original SME.

Once the single particle basis, single particle energies and the two-nucleon interaction is specified, one should construct the Hamiltonian matrix in the infinite dimensional Hilbert space and diagonalize it to get the eigen-energies and eigen-vectors for the valence nucleons wherefrom other nuclear properties can be calculated. However, infinite dimensional space is unmanageable. Therefore, one looks for a formalism wherein one may work in a manageably large subspace of the full Hilbert space and still get the same result as one would get in the

infinite dimensional space. This process of selecting out only few configurations to work with is called truncation and the truncated space as model space. Let us denote the full space by  $D$  and the model space by  $d$ . An operator  $\theta$  that describes a nuclear phenomenon in  $D$  will not do so in the same way if calculations are performed in  $d$  only. Hence the need of an 'effective' operator  $\theta_{\text{eff}}$  such that calculations with  $\theta_{\text{eff}}$  in  $d$  yield same results as one would get with  $\theta$  in space  $D$ .

Let us rewrite the basic equations in  $D$

$$\Psi = \sum_i^{\infty} a_i \phi_i$$

$$H_0 \phi_i = \epsilon_i \phi_i \quad i = 1, \dots, \infty \quad (1.16)$$

$$H = H_0 + V$$

$$H \Psi = E \Psi$$

We 'define' the model space wave function  $\Psi_d$  as

$$\Psi_d = \sum_{i \in d} a_i \phi_i \quad (1.17)$$

Let us define two projection operators:

$P$  operating on  $\Psi$  projects on to the space  $d$ :  $Q$  operating on  $\Psi$  projects onto rest of the Hilbert space. Mathematically,

$$P = \sum_{i \in d} |i\rangle \langle i| \quad (1.18)$$

$$Q = \sum_{i \notin d} |i\rangle \langle i|$$

However,  $P + Q = I$ , the identity operator.

Thus,

$$P|\Psi\rangle = |\Psi_d\rangle$$

We 'define' the effective Hamiltonian  $H_{\text{eff}}$  through

$$H_{\text{eff}} \Psi_d = E \Psi_d \quad (1.19)$$

We write from the set of equations (1.16)

$$\sum_{i \in D} a_i (H_0 + V) \phi_i = E \sum_{i \in D} a_i \phi_i$$

Multiplying on left with  $\phi_j^*$  and integrating over all space

$$\begin{aligned} (E - \epsilon_j) a_j &= \sum_{i \in D} a_i \langle \phi_j | V | \phi_i \rangle \\ &= \langle \phi_j | V | \Psi \rangle, \text{ for all } j \in D \end{aligned} \quad (1.20)$$

Although this equation is only a restatement of the original eigenvalue problem but it is important in this form in that it shows how one can do without both  $V$  and  $\Psi$ .

Let us define

$$V|\Psi\rangle = V_{\text{eff}} |\Psi_d\rangle \quad (1.21)$$

Then, eq. (1.20) can be interpreted to imply

$$(H_0 + V_{\text{eff}}) \Psi_d = E \Psi_d \quad (1.22)$$

Comparison with eq. (1.19) gives

$$H_{\text{eff}} = H_0 + V_{\text{eff}}$$

i.e. problem of calculating  $H_{\text{eff}}$  reduces to the one of calculating  $V_{\text{eff}}$ , the 'effective interaction'.

Let us see, how, using eq. (1.21),  $V_{\text{eff}}$  can be obtained from  $V$ .

$$\begin{aligned} V_{\text{eff}}|\Psi_d\rangle &= V|\Psi\rangle = V(P + Q) |\Psi\rangle \\ &= V|\Psi_d\rangle + VQ|\Psi\rangle \end{aligned}$$

Now,

$$\begin{aligned} Q|\Psi\rangle &= \sum_{\substack{j \notin d \\ i \in D}} |\phi_j\rangle \langle \phi_j | a_i | \phi_i\rangle \\ &= \sum_{\substack{j \notin d \\ i \in D}} |\phi_j\rangle a_i \langle \phi_j | \phi_i\rangle \\ &= \sum_{j \notin d} |\phi_j\rangle a_j \end{aligned}$$

$$\begin{aligned}
&= \sum_j \langle \phi_j | < \frac{\langle \phi_j | V | \Psi \rangle}{E - E_j} \quad (\text{using eq. (1.20)}). \\
&= \frac{Q}{E - H_0} V | \Psi \rangle = \frac{Q}{E - H_0} V_{\text{eff}} | \Psi_d \rangle
\end{aligned}$$

Hence,

$$V_{\text{eff}} | \Psi_d \rangle = V | \Psi_d \rangle + V \frac{Q}{E - H_0} V_{\text{eff}} | \Psi_d \rangle$$

or, in the operator notation

$$V_{\text{eff}} = V + V \frac{Q}{E - H_0} V_{\text{eff}} \quad (1.23)$$

i.e. given a two-nucleon potential  $V$ , the effective potential  $V_{\text{eff}}$  is obtained through an integral equation. We can see that  $V_{\text{eff}}$  explicitly depends on energy  $E$  which it is supposed to reproduce i.e. the effective interaction is state dependent. The state dependence may also include dependence on local density, centre-of-mass quantum numbers etc.<sup>7</sup>

Let us compare eq. (1.23) with eq. (1.15). The operator  $Q$  in eq. (1.15) allows scattering into unoccupied particle states only. In eq. (1.23), the operator  $Q$  is further restricted to allow the particles to be scattered outside the model space only. If one chooses only the lowest configuration as the model space, the effective interaction  $V_{\text{eff}}$  is completely equivalent to the reaction

matrix operator  $G$ . If model space consists of more than one configuration, to take into account configuration mixing, one has to diagonalize the matrix of effective Hamiltonian. Then, in eq. (1.15),  $Q$  can be thought of as made from two parts: one part allows scattering into model space and whose effect is treated by diagonalizing the reaction matrix in model space. However, the reaction matrix so formed within the model space should also incorporate the effects of the other part of  $Q$  which permits scattering outside the model space only. This process of modification of reaction matrix, calculated within model space, by happenings outside the model space, is called 'renormalization'. One, thus, sees that, in lowest order, when renormalization effects are ignored, the reaction matrix also represents effective interaction. Even otherwise if one exactly treats all the renormalizations, the  $G$  matrix is equivalent to the effective interaction. The unrenormalized  $G$  matrix is also often called the 'bare' interaction. Thus, one may use realistic interactions for spectroscopy calculations in finite nuclei provided one uses a reaction matrix and makes due allowance for renormalization effects.

Starting with a free  $N$ - $N$  interaction, Kuo and Brown<sup>8</sup> were the first to calculate the lowest-order

renormalization of reaction matrix. They obtained impressive agreement with experimental level energies using the renormalized interaction. Barrett and Kirson<sup>9</sup> then calculated the third-order contribution of core-polarisation process and they found that it almost cancelled the second-order contribution of Kuo and Brown. Kirson<sup>10</sup> has finally shown that infinite-orders sum of perturbation series for all hitherto physically conceivable renormalization processes is zero. We present detailed review of renormalization calculations in Chapter II.

Thus, starting from free N-N potential one may get good agreement with experimental data(as happened with Kuo and Brown) but one can not be certain if the reaction matrix has been correctly calculated and renormalizations properly treated although it is a matter of satisfaction that one knows the physical origin of the two-nucleon effective potential. In view of these uncertainties, one sometimes adopts a reverse approach. One knows a good deal about the qualitative character of N-N interaction. On

the basis of this one sets up a potential e.g. a potential of the form

$$V_{\text{eff}} = (a + b \vec{\sigma}_1 \cdot \vec{\sigma}_2) f(r)$$

incorporates the spin exchange character of the force.

The function  $f(r)$  determines the radial dependence of the potential and it will also contain the range of the force which may be taken to be spin-dependent. The parameters (a, b and force range appearing in  $f(r)$  in above example) of such a potential are determined by requiring that experimentally observed properties of the nucleus under consideration, e.g. its energy levels, are reproduced. Sometimes one also adopts Talmi approach<sup>11</sup> wherein the two-body matrix elements themselves are parameterized. Effective potentials derived in this way are termed 'phenomenological'.

## I.2 PROBLEMS FOR PRESENT WORK:

(i) Except for a few unavoidable practical limitations, the N-N force in free space is very well known. However, it can be realized at the outset that a free N-N interaction will not also describe the situation inside a bound nucleus for the obvious reason that the free N-N force would be modified by presence of other nucleons. In case of phenomenological effective potentials the core part is assumed to be inactive and parameters are forced to reproduce experimental numbers. In case of free N-N interaction we do not have any free parameter at our disposal which might be forced to attain some value so as to reproduce experimental facts. Therefore, with a free N-N interaction between valence nucleons, their



interaction with core nucleons can not be ignored. Further, an infinity of final states is available when two particles scatter in free space. Within bound nucleus, they move in quantized orbits. Yet, while initially in a given quantum state, they can scatter into any of higher unoccupied orbits. In principle, they are also infinite in number. Due to our inability to handle infinite dimensional matrices we have to define a model space. Again, parameters can be forced to get a phenomenological effective interaction but with realistic interactions, some analytical mathematical formalism has to be developed to incorporate both core effects and effects of outside-of-model-space configurations i.e. the free N-N interaction needs to be properly renormalized. Kirson<sup>10</sup> has finally shown the inadequacy of present microscopic calculations for estimation of renormalization corrections. Schucan and Weidenmüller<sup>12</sup> believe that the failure of purely microscopic approach lies in the fact that in this approach the theory is completely isolated from experimental results for bound states, except that the free N-N interaction is also most generally derived to fit to bound state properties of deuteron, and at no stage of calculation do we know where our calculations are directing us to. However, this does not mean that things

are wrong with theory, of course, there are always practical limitations, but only that the true renormalization process has yet to be discovered. So long as we do not know that process and mathematical formalism to handle it, we can at least deduce in a much simpler way the amount of renormalization needed by introducing phenomenological and experimental information into calculation so that at least the qualitative nature of the renormalizing force may be understood although it is rather definite that once we come down to phenomenology, there can be more than one ways of achieving the same final effect on mathematical numbers and we do not claim the uniqueness of phenomenology we plan to introduce.

At least one thing is obvious from the results obtained by so many people working with realistic interactions that the derivation of reaction matrix itself, starting from a free N-N potential, is one of major causes of uncertainties. In view of this, the Sussex matrix elements (SME) present a favourable situation in that the reaction matrix needs not be derived. Previous calculations<sup>13</sup> have shown that bare SME are not sufficient to describe bound state nuclear properties i.e. there is a need to renormalize them. However, we do not adopt a microscopic approach for calculation of renormalization corrections. The SME are available as numbers and the

exact form of the free N-N potential which they represent is not known. If we were to adopt microscopic approach for renormalization it would be only numbers for relative matrix elements which would be needed but to decide for the phenomenology to be adopted, the behaviour of interaction towards different nuclear properties should be known. Assuming the potential to be smooth and a combination of central, spin-orbit and tensor parts, we, therefore, first decompose the SME into matrix elements of component interactions and study the effect of each component on low-energy spectra of two -valence-nucleon nuclei  ${}^6\text{Li}$ ,  ${}^{18}\text{F}$ ,  ${}^{18}\text{O}$ ,  ${}^{42}\text{Sc}$ ,  ${}^{42}\text{Ca}$ ,  ${}^{58}\text{Ni}$  and  ${}^{92}\text{Zr}$ .

Comparison of these spectra among themselves and of each with experimental one will help in assessing the importance of individual components. It will be helpful in deciding the phenomenology to be adopted. This way, we will end up with an, we can call it semi-phenomenological or semi-realistic effective interaction and the approach lies somewhere between purely microscopic approach to calculation of renormalization corrections and a totally phenomenological parameterization of effective two-nucleon interaction - let us call it semi-microscopic. We discuss this problem in Chapter II.

(ii) The next problem is that of the isotones  ${}^{40}\text{K}$  and  ${}^{38}\text{Cl}$ . Today, we have enough experimental data

regarding levels of  $^{40}\text{K}$ . Paucity of enough experimental data has always been realized as the biggest block in the way of establishing a reasonable phenomenological effective interaction. Moreover, generally even the low-lying nuclear levels contain quite complicated components in the wave function so that parameterization of a phenomenological effective interaction in a model space of simple configurations is always doubtful. In view of these difficulties, the  $^{40}\text{K}$  nucleus presents quite favourable a situation since it had been realized as back as in 1956 by Goldstein and Talmi<sup>14</sup> that low-lying states of this nucleus are almost pure configurations. Moreover, about 9-10 low-lying levels of  $^{40}\text{K}$  have well established energies and spins and therefore parameterization of a phenomenological effective interaction comprising of central, spin-orbit and tensor dependences can be adventured with much less stringent approximations. However, the available experimental information for  $^{40}\text{K}$  is just sufficient for determination of parameters of an effective interaction consisting of a central, a two-body spin-orbit and a tensor part. To check their validity, the most immediately calculable thing is the spectrum of  $^{38}\text{Cl}$  through the use of Pandya transformation<sup>15</sup>. We discuss this problem in Chapter III.

(iii) In the above mentioned two problems we attack the problem of establishing effective interaction from two different corners. There are few yet undecided factors which decide the nature of a true N-N interaction may it be either a phenomenological effective interaction or the one derived from a realistic two-nucleon interaction. However, the work of Cohen et.al.<sup>16</sup> on pseudonium nuclei showed that one could adopt a smaller model space and yet obtain an effective interaction by simply an adjustment of parameters that the 'pseudo experimental' data are excellently reproduced. On the other hand, Gupta and Trainor<sup>17</sup> proved that this result had no generality and nuclear properties dependent on wave functions e.g. electromagnetic transition rates could still <sup>be</sup> relied upon as sensitive test to 'goodness' of an effective interaction.

Schucan and Weidenmuller<sup>12</sup> have shown that, a priori, there is no reason to expect that the perturbation expansion for  $V_{\text{eff}}$  converges. Nonconvergence means that we are trying to calculate too strong effects in perturbation theory. We renormalize a free N-N interaction to take into account configurations neglected from being included in the model space. Nonconvergence would then imply that such strongly contributing configurations should be explicitly included in the model space. This

is not the realization of facts for the first time but it has always been avoided on the plea of otherwise increased computational difficulties. We study this problem of truncation of configuration space for  $^{42}\text{Sc}$  nucleus for a randomly chosen two-body central potential, however, keeping in mind that the approximate numerical results given by this set are not orders of magnitude off the experimental results so that the qualitative results we plan to extract do not turn out to be completely hypothetical. We first study the separation between centroids of  $T = 1$  and  $T = 0$  states arising from  $(0f_{7/2})^2$  configuration as a function of the four  $A_{TS}$  strength parameters and space dimensionality. This is done with a view to assess the relative importance of even and odd  $\ell$  partial waves in nuclear structure calculations. This study is expected to be useful since, at times, the use of a Serber force<sup>18</sup> or just a central, S-state interaction<sup>19</sup> has been tried for calculation of two-body spectra. This study will then tell us the limit in which such an approximation can be used that we altogether drop the odd  $\ell$  part of the interaction.

There is no a priori reason to believe that all configurations within a model space contribute equally and a particular configuration within the usually chosen model space might be contributing just negligibly in

comparison to other configurations within the same model space. This study is expected to be useful for a more honest calculation of shell model effective interaction in the sense that if some of the usually chosen potential parameters and configurations can be established to contribute much less than others then they can as well be dropped out and an equal number of parameters and configurations can be included in the calculation, which would otherwise have to be excluded in view of computational difficulties and which can be proved to have more pronounced effect - just without adding to computer time. We study this problem in Chapter IV.

## CHAPTER II

### PHENOMENOLOGICAL ESTIMATION OF RENORMALIZATION CORRECTIONS TO FREE NUCLEON-NUCLEON INTERACTION

#### II.1 INTRODUCTION:

Before one makes nuclear spectroscopy calculations, one has to decide for the effective interaction one wants to work with. There are two choices open-phenomenological effective interaction or an effective interaction derived from free nucleon-nucleon (N-N) interaction. Each one has its own merits and demerits.

Suppose we choose some phenomenological form. We may not be sure whether we have included all the required features of a true N-N potential. Suppose, we assume a central force. Then, we are ignoring, say, spin-orbit and tensor forces, whose effects, we may not know beforehand, might be important. Suppose we include them also. Then, we might still be missing some other features, say hard core. In principle, we can incorporate as many features as we wish while formulating an interaction but we have to remember that each time we include a new component, we add at least one more parameter and



the limit to number of parameters, which can be determined, is set by the amount of available information. We have seen in Chapter I that one mostly finds the unknown parameters by making fit to experimental excitation energies and one, at least, requires as many excitation energies as the number of parameters. Such a calculation is feasible only if the needed energy levels also have well defined spin and parity. Our knowledge of experimental energy levels is not rich enough and not many levels have unambiguously established spin and parity, even in the low energy region. This means that one can gain only a limited description of the effective potential.

Even if enough experimental data is available, it is very important in these calculations that one should be able to assign a reasonable configuration to an experimental level so that it may be meaningful to compare the matrix element calculated for that configuration, with the level energy. It often happens that, for example in two-valence-nucleon nuclei one observes a very low-lying  $0^+$ ,  $T = 1$  excited level which cannot be explained on the two-particle shell model<sup>20</sup>. Instead, it has been shown to be a core-deformed four particle-two hole (4p - 2h) state<sup>21</sup>. With a core-excited state getting down so much low in energy, one may legitimately

question the purity of other nearby levels in respect of shell model configuration. In view of such ambiguities, it is no surprise that for same nucleus one often ends up with two completely different sets of parameters which reproduce the energy levels equally well. An example is found in ref. 22 where it is shown that different sets of parameters give equally good fit to doublet splitting in  $A = 14$  and  $A = 16$  nuclei.

To avoid these difficulties in constructing a phenomenological form for potential, one may decide to adopt the Talmi method. Again, the paucity of enough experimental information comes in the way. However, one has a way out. One picks up a set of nuclei in the same shell e.g. one might select all nuclei with  $A = 18$  to 20 for determination of effective interaction in sd-shell<sup>23</sup>. Matrix elements for configurations of more than two valence nucleons can be expressed as linear combinations of two-body matrix elements. One makes the assumption that the two-body matrix elements do not change in magnitude in neighbouring mass number nuclei of the same shell. Thus, one parameterizes the two-body matrix elements simultaneously for a series of nuclei. However, such calculations have to be restricted to a very small model space just because one may not be able to

assign reasonable configurations for all the energy levels even if all of them have well established spin and parity. One is thus constrained to assume that configurations lying outside the model space are either ineffective or their effect has been absorbed in the calculated values of the two-body matrix elements. Unless one establishes that effects of left out configurations are negligible, one can only infer that, alright, the matrix elements represent those of an effective interaction but it may not be fair to say that numbers so obtained are representative of 'true' N-N force. Obviously, such calculations are strongly space dependent. Further, one is making a total neglect of many-body effects. One is assuming that the two-body interaction in a many-valence nucleon configuration is not altered by presence of other nucleons from a value it is in a two-valence nucleon system and that three-or more-body forces are not present. Suppose, we had enough knowledge so that even in this approach we were able to find the effective interaction separately for different nuclei. Then, if the two-nucleon interaction is altered by presence of other nucleons or if more-than-two-body forces themselves are important, it will be reflected in the calculated values of the effective two-body matrix elements.

One makes a simplification over this method. Every two-body matrix element, diagonal, off-diagonal or of any configuration, is basically a linear combination of relative matrix elements. The relative matrix elements themselves stay constant in all two-body matrix elements for a given nucleus; geometry of the matrix element only alters the coefficients of the aforementioned expansion. Therefore, one tries to parameterize the relative matrix elements<sup>19,24</sup>. Within a given major shell, only a finite number of relative matrix elements appear. This way, one requires much less experimental data than in Talmi approach.

This approach is further simplified by one's knowledge about the nuclear forces. One knows that nuclear forces are short ranged. Hence, it may be a good approximation to ignore interaction in states with  $\ell > 2$  since in higher partial waves the nucleons are not allowed to get close enough due to increased centrifugal repulsion. One may further assume the existence of central forces only in which case, for example, the  ${}^3P_0$ ,  ${}^3P_1$  and  ${}^3P_2$  relative states are degenerate. People have gone upto the extent of neglecting even P- and D - partial waves. Interaction in P-states can be ignored on the plea that forces are much weaker in odd- $\ell$  states. Neglect of D-state interaction is justified by saying

that it will be much weaker than the leading S-state term and that once we are all out to determine an effective interaction only, let their small effect also be absorbed in the effective interaction parameters. One should, at least, include the strong  ${}^3S_1 - {}^3D_1$  tensor force but this force only renormalizes the triplet state interaction and so it is also included in the triplet-state central interaction. Like this, one is able to reduce the number of free parameters drastically but only at the expense of losing details about the structure of the N-N potential.

After the relative matrix elements are thus determined, one may attempt at interpreting them in terms of an effective potential and find the strength and range of the potential.

Above discussion makes it clear that an effective interaction, phenomenological atleast, cannot be unambiguously established. In fact, the numbers depend upon which configurations one is considering and which nuclear properties one wants to reproduce. Since most of the attempts are aimed at reproducing energy levels, wave functions are never guaranteed and hence no guarantee that wave functions will be good enough so as to reproduce other nuclear properties also equally well.

Due to difficulties in determination and uncertainties in results obtained for an effective interaction, one looks for some alternative approach wherein the potential appears as a natural consequence rather than a forcible introduction to reproduce experimental data. One has a good knowledge of N-N interaction in free space; one tries to employ it for calculation of bound state properties of nuclei.

One is required to calculate matrix elements of the interaction. Therefore, if the interaction possesses a hard core, one should first of all calculate the reaction matrix

$$G = V + V \frac{Q}{E - H_0} G \quad (2.1)$$

However, it should be remembered that a reaction matrix which is representative of N-N interaction in free space will not describe the N-N force inside a bound nucleus also. Probably the best example in support of this statement is: in free space, neutron has a half-life of about 12 minutes but inside a bound nucleus it stays permanently as neutron! Certainly the interaction of a neutron with other particles when inside a nucleus is different from the interaction with same particles in

free space. To the extent that core could be considered as inert, the reaction matrix itself will be effective interaction in infinite dimensional Hilbert space of valence nucleons. However, the idea of infinite dimensional space is not practical and further, the concept of effective interaction itself is associated with a model space. Let us see what form does eq. (2.1) take when the full Hilbert space is partitioned into two subspaces. Let,  $\mathcal{Q} = \mathcal{Q}_1 + \mathcal{Q}_2$  where  $\mathcal{Q}_1$  allows scattering into model space only and  $\mathcal{Q}_2$  allows them to be scattered into any not-already-occupied state. Assuming the outside-of-the-model-space effects to be small enough so that retention of only those terms where  $\mathcal{Q}_2$  appears only once is a good approximation, the expansion on right of eq. (2.1) can be grouped to give

$$G \simeq G_1 + G_1 \frac{\mathcal{Q}_2}{E - H_0} G_1 \quad (2.2)$$

where  $G_1$  is the reaction matrix generated within the model space

$$G_1 = V + V \frac{\mathcal{Q}_1}{E - H_0} G_1 \quad (2.3)$$

However, a complete expansion gives

$$G = G_1 + G_1 \frac{Q_2}{E - H_0} G \quad (2.4)$$

This means that if one wants to work in a model space, one will have to iterate over the reaction matrix calculated in the model space. How many higher orders will be required in order to get congruence with experiment will depend on how good is the description rendered by  $G_1$  itself.

In the present work we have adopted a semi-microscopic approach to derive effective interaction. What persuaded us to take such a step has been the fact as observed by others that even with the present day computers that application of more and more sophisticated calculational techniques has been possible, we do not yet have a satisfactory theory for nuclear structure physics. Our attempt has been to see if we can understand the N-N force in a simpler way. To make a case for ourselves (in defence of our simple minded approach over much more involved calculations of others) it will be in order that we review as to ultimately what has been the fate of an almost uncountable number of calculations employing purely microscopic approaches.



Historically, first attempt of calculating reaction matrix for an open shell finite nucleus was made by Dawson et.al.<sup>25</sup> They used the PGT potential<sup>26</sup> and made calculations for  $^{18}\text{O}$  nucleus by diagonalising the reaction matrix in sd-shell. The ordering of first five states was correctly reproduced and the level energies were roughly reproduced. In the lowest approximation when the reaction matrix was approximated by the interaction itself, it was clearly seen that on expanding the space from  $(\text{Od}_{5/2}, 1s_{1/2})$  to  $(\text{Od}_{5/2}, 1s_{1/2}, \text{Od}_{3/2})$ , the results turned out to be in better agreement with experiment. The results further improved when the reaction matrix also included  $2\hbar\omega$  intermediate states. Although the gross features one could conclude were that the ground state was predicted at a higher energy than experimental value and the calculated spectrum was too compressed, yet the results pointed towards a brighter future for such calculations provided one makes a more careful calculation of the reaction matrix and assumes a large enough model space.

It is for one's own convenience that there not be a mess of computation that one assumes the core as inert. Results of Dawson et.al. proved that the reaction matrix is not weak enough to retain particles within the model

space only. Besides being scattered into outside the model space, they could also interact indirectly - via the mechanism of core excitation. This process represents a long-range correlation which is produced by short-range interactions. Classically it can be viewed like this: one of the two nucleons, particularly on the surface of a large nucleus, interacts with a core-nucleon and excites it to some empty orbit, thus creating a particle-hole pair. Then, the other valence nucleon interacts with the excited nucleon and throws it back in the created hole. In terms of diagrams, the process, in which two nucleons in the state  $|ab\rangle$ , while interacting via core-excitation, are scattered into the state  $|cd\rangle$ , is represented as shown in Figure 2.1a. In this diagram, a, b, c and d are particle states within the model space. Clearly, the intermediate states in this process are those of three particles and one hole ( $3p-1h$ ). This correction to the reaction matrix is denoted by  $G_{3p1h}$ . It can be noted that to conserve parity, the core-nucleon can only be excited by  $2n\frac{1}{2}\omega$  ( $n = 0, 1, 2, \dots$ ) single-particle energy. The special case of  $n=0$  occurs when the core is formed by shell closure in the middle of a major shell e.g. the  $^{58}_{28}\text{Ni}$  nucleus. The core is  $^{56}\text{Ni}$  with both neutron and proton shells closing at  $\text{Cf}_{7/2}$  and the two valence neutrons being in the  $1p_{3/2}$

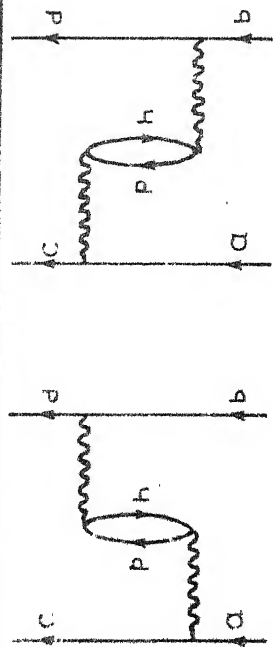


FIG. 2.1a. ONE PARTICLE-ONE HOLE RENORMALIZATION OF REACTION MATRIX

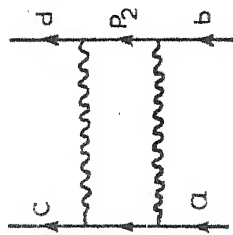


FIG. 2.1b.  $G_{2p}$  RENORMALIZATION OF REACTION MATRIX

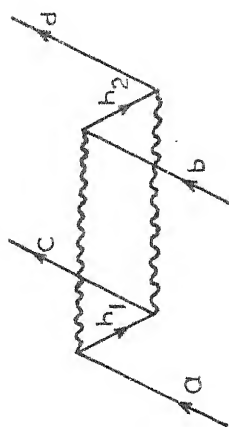


FIG. 2.1c.  $G_{2h}$  RENORMALIZATION OF REACTION MATRIX

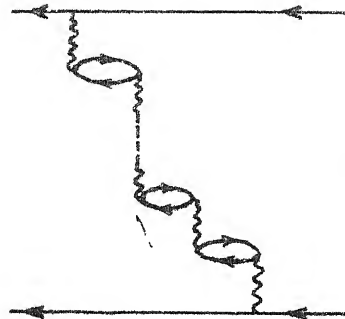


FIG. 2.1d. TDA RENORMALIZATION OF REACTION MATRIX

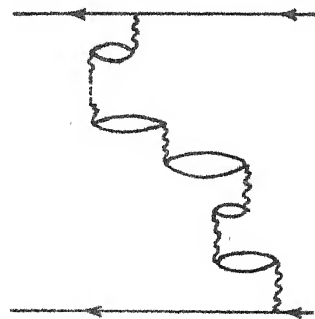


FIG. 2.1e. RPA RENORMALIZATION OF REACTION MATRIX

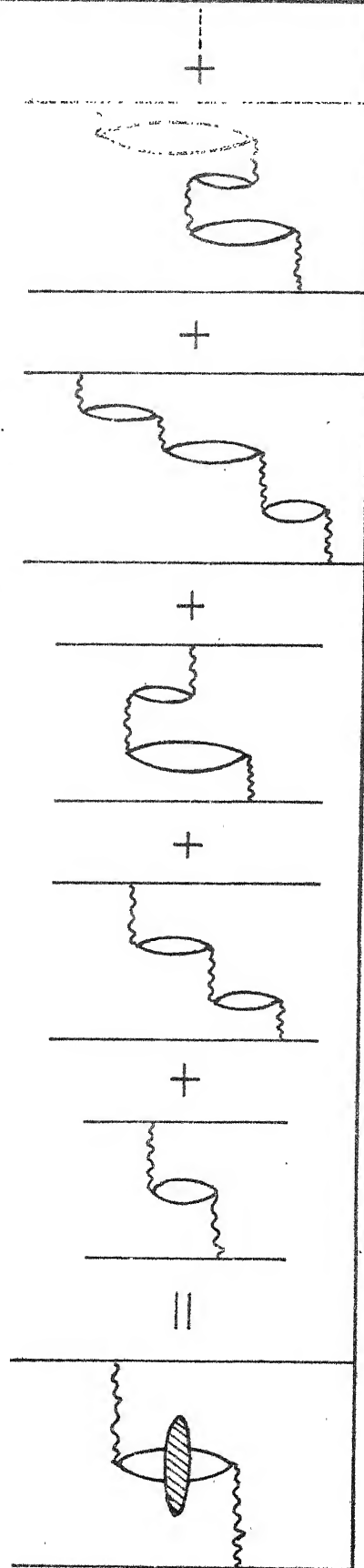


Fig. 2.1f. Infinite orders sum of TDA and RPA series for renormalization of reaction matrix

orbit. The parity requirement does not forbid a  $0f_{7/2}$  nucleon to be lifted to any of the orbits  $1p_{3/2}$ ,  $0f_{5/2}$  and  $1p_{1/2}$ .

Let us see, mathematically how the contribution of such a physical process can be calculated. In the original derivation of reaction matrix, eq. (2.1), the Pauli operator  $Q$  was designed to allow scattering into particle states only. In fact, the introduction of this operator is necessitated by the requirement that the particles not be allowed to be scattered into occupied states. The idea of core-excitation was not conceived at that time. The above decomposition of  $Q$  into  $Q_1$  and  $Q_2$  and eventual arriving at eq. (2.4) should be valid if, apart from two-particle intermediate states,  $Q_2$  also incorporates others: renormalization processes which do not violate Pauli principle e.g. the core-excitation process. Henceforth we drop the subscript 1 on  $G_1$  with an understanding that the reaction matrix is being calculated in a model space. Then, the lowest-order correction, second-order in  $G$ , to the bare  $G$  matrix will be

$$G_{3p1h} = G \frac{Q_{3p1h}}{e} G$$

where  $e$  is the appropriate energy denominator and

$$Q_{3p1h} = \sum_{ph} |3p1h\rangle \langle 3p1h|$$

It was first of all pointed out by Bertsch<sup>27</sup> that the core-polarisation process has the useful property of lowering energy levels of low  $J$  and raising those of high  $J$ . It is just the desired effect: the calculated ground state will be in better agreement with the experiment and the compressed spectrum will spread up. Importance of core-excitation process is indicative of importance of dynamic effects of the core after the static effects have been eliminated by factoring out the core energy.

Similarly, the correction arising from two-particle intermediate states (Figure 2.1b) is calculated as

$$G_{2p} = G \frac{Q_{2p}}{e} G$$

$$Q_{2p} = \sum_{2p} |2p\rangle \langle 2p|$$

In Figure 2.1b, both  $p_1$  and  $p_2$  are particle states outside the model space. Owing to the intermediate-state energy occurring in the denominator, it is expected that, except for the particular case where intermediate state excitations into same major shell are possible like in  $^{58}\text{Ni}$ , intermediate states with single particle excitation energy  $2\hbar\omega$  will be most important.

We have considered the process where one core-nucleon is raised through  $2\hbar\omega$  energy. However, energy-wise it should be equally probable that two core nucleons from just below the Fermi surface are lifted, each by  $\hbar\omega$ , into the model space. In this process, intermediate states are of four particle-two hole (4p2h) character. This correction is represented as in Figure 2.1c and denoted by  $G_{2h}$ .

Thus, the total, renormalized interaction becomes

$$G + G_{3p1h} + G_{2p} + G_{2h}$$

Kuo and Brown<sup>8</sup> applied these ideas to structure calculations of  $^{18}\text{O}$  and  $^{18}\text{F}$  nuclei starting from Hamada-Johnston (HJ) potential<sup>28</sup>. They first calculated the spectra with bare  $G$  interaction. The results were nowhere in agreement with experiment thus confirming the necessity of renormalizations. However, they included only the  $G_{3p1h}$  correction. They did not have to go beyond lowest order correction (second-order in  $G$ ). In the second-order itself, the agreement with experimental spectra was satisfactory. It was natural to think that third - and higher-order corrections all cancel among themselves.

Kuo and Brown neglected the  $G_{2p}$  correction on the grounds that it is essentially a second-order ladder

diagram and hence its effects are already included in the calculation of reaction matrix,

However, energy levels are a crude test of the effective interaction and they, infact, failed to reproduce E2 transition rate from second  $0^+$  state to first  $2^+$  state. These states are usually believed to be deformed, containing 4p-2h core-excited component. However, they were able to reproduce reasonably well, energies of these levels as two particle states with 3p1h corrections. The plea that they gave for neglect of  $G_{2h}$  correction was that the 4p-2h deformed states are highly collective and hence are much lowered in energy and so it will not be proper to calculate the  $G_{2h}$  correction in perturbation theory taking a  $2\hbar\omega$  energy denominator. This neglect thus showed up in the transition rate.

The Kuo-Brown G matrices were recalculated by Kuo<sup>29</sup> using the same intermediate states assumptions but treating the short-range repulsion of the interaction and the state dependence of the second-order tensor term more carefully. His results for G and  $G_{3p1h}$  were significantly different from those of Kuo and Brown and this destroyed the good agreement with experiment they had earlier. Kuo, therefore, incorporated the  $G_{2p}$  and  $G_{2h}$  corrections also and this improved the fit.

Since the first successful calculation of core-polarisation correction by Kuo and Brown, there have been a large number of calculations<sup>30-34</sup> starting from a free N-N interaction. These calculations have been performed with either  $G + G_{3p1h}$  or  $G + G_{3p1h} + G_{2p} + G_{2h}$ . They all substantiate the original findings of Bertsch that the bare interaction does not give satisfactory agreement with experiment and even philosophically it is wrong to make comparison with experiment at this stage. The ground state energy is not correctly reproduced and the calculated spectrum is too compressed. However, inclusion of core-polarisation lowers the calculated ground state and also causes an overall spreading in the spectrum thus bringing it in better agreement with experiment.

Thus, although reasonable agreements with experiment were obtained but from a theoretical viewpoint it was a disturbing feature that the theory did not provide a unique prescription for calculation of reaction matrix and for number of terms to be kept. For example, Kuo and Brown got impressive agreement with  $G + G_{3p1h}$  but when Kuo did an improved calculation of  $G$ , he had also to include  $G_{2p}$  and  $G_{2h}$  corrections to restore the agreement.

Even Kuo and Brown had realized that it might not be sufficient to include just one-bubble term in the treatment



of core-excitation. Instead, one should calculate it as a series of forward going bubbles (known as TDA) shown in Figure 2.1d or, as a series of both forward and backward going bubbles (known as RPA) shown in Figure 2.1 e.

Thus, the total interaction should be as shown in Figure 2.1 f. where the hatched circle on left means a summation of series of diagrams on right. A series of particle-hole pairs created one after the other constitutes what is known as a 'phonon'. The reason why the interaction among valence nucleons should be renormalized by a phonon and not by a single bubble is that some of these phonons may be highly collective and thus much lowered in energy and then taking  $2\hbar\omega$  as energy denominator would be much undermining its contribution. They<sup>8</sup> argued, however, that some of these particle-hole states will be spurious and they should come at zero energy. Further there is every chance that several of these phonons will lie much higher in energy. Hence, they thought it legitimate to include just one bubble correction.

As more and more core-polarisation calculations were made, it became clear that the first-order corrections (second-order in  $G$ ) had a large effect on spectra and in some cases the second-order correction was even larger

than the bare interaction  $G$  itself. One, then, becomes suspicious whether or not are the third-and higher-order corrections actually negligible.

An attempt to incorporate the strings of bubbles introduced above was first made by Kuo<sup>35</sup>. He constructed the core-polarization phonons in RPA and included their effect by coupling them to the valence particles in  $A=18$  nuclei. He observed that low-lying spectra calculated with  $G + G_{\text{phonon}}$  and  $G + G_{3p1h}$  were quite similar. Hence, he concluded that to calculate the core-polarisation effects involving exchange of positive parity phonons it is sufficiently accurate to calculate the effect in first-order theory itself i.e. include just the  $G_{3p1h}$  correction although calculation with phonons is desirable.

An arithmetical error in Kuo's calculations was discovered by Osnes and Warke<sup>36</sup> who repeated the RPA calculations for  $A = 18$  nuclei and concluded that significantly different results for renormalization of the two-nucleon effective interaction are obtained depending on whether the core-excitations induced by the valence nucleons are represented by single unperturbed particle-hole excitations or by the full RPA solutions for the core.

Since then a trend has set up for calculation of core excitation corrections to effective interaction

between valence nucleons in TDA and RPA. Zamick<sup>37</sup> concluded that the core-polarisation calculated in RPA is much larger than the one in second-order perturbation theory. Ellis and Siegel<sup>38</sup> explicitly summed to second- and all-orders the perturbation theory diagrams of the TDA and RPA for renormalization of effective interaction between two sd-shell valence nucleons. They demonstrated the equivalence of infinite sum to the method of construction of phonons and observed large enhancements compared to the first-order perturbation correction. This equivalence has been demonstrated again by Goode and Kirson<sup>39</sup>. Starting with Kallio-Kolttveit (KK) interaction<sup>40</sup>, Siegel and Zamick<sup>41</sup> have observed the same enhancement in respect of effective charge for closed shell  $\pm$  one nucleon nuclei. In fact, for certain choices of G matrix elements, the enhancement is infinite<sup>38</sup>. Kirson and Zamick<sup>42</sup> have named this process 'propagator renormalization'. All these calculations end up with the conclusion that strong collective enhancement occurs when these series are summed up and that, in particular, the ground states are depressed far below the experimental energies. It, then, became clear that some compensating effect was needed to off-set this negative enhancement. Osnes et.al.<sup>43</sup> have repeated these calculations for

valence nucleons in fp-shell. They also find that the difference between RPA and one-bubble descriptions is much larger for fp-shell valence nucleons than for sd-shell ones. A possible explanation for this difference is that the  $^{40}\text{Ca}$  core is much bigger than the  $^{16}\text{O}$  core thus allowing a larger number of intermediate states.

Brueckner's idea behind introduction of reaction matrix was that after all singularities are treated out, the resulting G matrix will be weak enough that meaningful calculations could be performed in a model space or at most one would require one or two lowest-order corrections. However, the inadequacy of bare G interaction and largeness of second-order corrections had necessitated investigation of third- and higher-order corrections. Therefore, at the same time that above mentioned RPA corrections were started, Barrett and Kirson undertook the calculation of third-order correction for  $A = 18$  nuclei using Kuo reaction matrices derived from HJ potential. In a preliminary note<sup>44</sup> they observed that there is no evident term-by-term convergence when the core-polarisation is treated in perturbation theory. Instead, an analogy with Bethe's nuclear matter results<sup>45</sup> suggests that the core-polarisation is so strong that it cannot be treated by perturbation theory at all but must be handled by a method which sums perturbation theory to all orders.

They, then, reported<sup>9</sup> the results of their calculations to their-order and also of a few selected terms to fourth-order which contribute to the perturbation series for  $O^+$ ,  $T = 1$  effective interaction between valence nucleons in  $A = 18$  nuclei. They found the total third-order correction to be as big as or bigger than the second-order contribution. They, thus, concluded that there is no apparent convergence in the perturbation expansion for  $V_{\text{eff}}$  in powers of  $G$ . However, they did observe that the contribution of  $4p - 2h$  correction in third-order was an order of magnitude smaller than the corresponding number in second-order. It was, thus, safe to conclude that no collective enhancement is produced by this type of correction. This conclusion is consistent with that of Goode<sup>46</sup> and Rajewski and Kirson<sup>47</sup> who have summed this effect to all orders in  $G$  and found little or no enhancement. Barrett and Kirson<sup>48</sup> also performed calculation for the simplest third-order number conserving set of diagrams which represent the renormalization of the bare reaction matrix for  $A = 18$  nuclei. The sum of terms within this set was found to be small, being 10 per cent of  $G$  or less.

There is double-counting involved when  $G_{2p}$  correction is included in third-order. Although the exact amount of this double-counting is uncertain, it has been

shown by Kirson<sup>49</sup> that the inclusion of two-particle ladders in an expansion in terms of the Kuo  $G$  matrices creates a double counting which can be as big as 100 per cent. For this reason, Barrett and Kirson had not included the  $G_{2p}$  correction in their third-order calculations. Barrett<sup>50</sup> has attempted to determine the size of this double counting by comparing the Kuo  $G$  matrix elements with the Barrett et.al.<sup>51</sup> (BHM) reaction matrix elements. He finds that the amount of overcounting depends strongly on the size of the gap between occupied and unoccupied states in the single particle energy spectrum in the calculation of the BHM reaction matrices, being largest for a small gap. In spite of the overcounting problem which occurs, it has been suggested<sup>52</sup> that two-particle ladder terms should be included in the expansion for  $V_{\text{eff}}$  computed with the Kuo  $G$  matrices. It has also been argued<sup>52</sup> that the third-order RPA diagrams should be included even though these diagrams contain excitations of  $4\hbar\omega$  and are not a pure  $2\hbar\omega$  contribution. In view of these suggestions, Barrett<sup>53</sup> recalculated the third-order correction with two-particle ladder terms and RPA diagrams included. The results weakened his earlier conclusion regarding nonconvergence of the perturbation expansion for  $V_{\text{eff}}$  although he still maintained that the prospects of improved convergence were questionable in view of overcounting problem.

In the same model space (sd-shell), Goode and Koltun<sup>54</sup> have shown that the (JT) - weighted average of the perturbation theory terms is repulsive in third- as well as in second-order. Therefore, the conclusion of Barrett and Kirson that second-and third-order terms cancel for  $0^+$ ,  $T = 1$  levels cannot be generalized to other JT states. Goode<sup>55</sup> has performed calculations for  $A = 18$  nuclei for all JT states in sd-shell. He concludes that with the possible exception of  $0^+$ ,  $T = 1$  levels, the calculated spectra are quite similar whether calculated in second-or in third-order perturbation theory although the spectra calculated with  $V_{\text{eff}}$  calculated upto second- or upto third-order terms are much different from the ones with bare reaction matrix. Grossly, it can be said that third-order effects on the  $T = 1$  states tend to be small compared to corresponding second-order effects. However, this is not quite the case with the  $T=0$  states where evidence for nonconvergent behaviour is found, probably due to manifestation of the tensor part of the N-N interaction. The  $T = 0$  spectra calculated in first, second-and third-order perturbation theory are quite different. In particular, the most dramatic third-order effects occur for the lowest  $1^+$  and  $2^+$ ,  $T = 0$  states each of which lies about 1 MeV higher when third-order correction is applied than when only second-order

effects are included. It appears that the two-lying experimental  $T = 0$  spectrum of  $^{18}\text{F}$  is better represented in second-order perturbation theory than in third-order.

Although Barrett and Kirson had proved a term-by-term nonconvergence of perturbation series in  $G$ , yet they had suggested that it might be possible to rearrange the perturbation series into physically significant groups of diagrams so that each group converges order-by-order in  $G$ . However, one must then find some way to sum all these groups of diagrams. Otherwise, as such, simple perturbation theory does not seem to be a reliable method for calculating the effective two-nucleon interaction when currently standard calculation techniques are used.

It was suggested by Kirson and Zamick<sup>42</sup> that for calculating  $V_{\text{eff}}$  between valence nucleons, one should also renormalize the interaction between the valence nucleons and the core. This was referred to as vertex renormalization and it was suggested that it should also be summed to all orders. They calculated the modified vertex to second-order in  $G$ , included it in the RPA and found that the resulting vertex renormalization tended to cancel the propagator renormalization. They also found that the multipole structure of the renormalization was more complicated than that given by a pairing or a pairing-plus-quadrupole interaction.



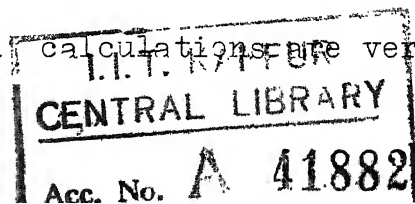
There is no reason why the particle-hole interaction should not be renormalized by the core as well. This process was called 'screening' of the particle-hole interaction. Core renormalization of the particle-hole interaction with various potentials has been considered in refs. 56-61. Blomqvist and Kuo<sup>62</sup> employed HJ interaction for calculation of negative parity particle-hole excitations of  $^{40}\text{Ca}$  and  $^{48}\text{Ca}$  with and without including the core-polarisation. Lowest  $3^-$ -states were found to be very sensitive to the core-polarisation. The RPA with the bare  $G$  interaction overestimates the collectivity of these  $3^-$ -states. The inclusion of self-screening diagram largely reduced the collectivity and the final result was quite similar to the TDA solution with bare  $G$  interaction. It must be kept in mind that  $^{40}\text{Ca}$  or  $^{48}\text{Ca}$  are big cores and allow many more particle-hole excitations than does a smaller core say  $^{16}\text{O}$ . However, if one can establish the same fact-that 'renormalized RPA' solution is as good as 'bare TDA' one - for other cases as well, one has obtained a much simpler way of dealing with core-excitation phonons-TDA with bare particle-hole interaction. Since the screening of the particle-hole interaction so greatly affects the collectivity of the core states, it must, in turn, be expected to be important for core-polarisation of the particle-particle interaction<sup>63</sup>.

Kirson<sup>10</sup>, then, undertook to sum the RPA series, the vertex renormalization series and the self-screening diagrams to all orders in  $G$  and found that the net result of these three infinite series taken together was approximately zero. The TDA and RPA series greatly depress the spectrum. The inclusion of screening damps the RPA back to TDA. Finally, the inclusion of the vertex or black box renormalization produces a spectrum which looks like that for the bare  $G$ . Kirson<sup>64</sup> has recently incorporated one more effect neglected in his earlier calculations, namely, the phonon-mediated screening of the vertex connecting zero-particle, zero-hole states of the core to two-particle, two-hole states. He concludes that core-polarisation, when self-consistently treated is too weak to account for significant renormalizations required for the  $^{16}\text{O}$  core, whether applied to particle-particle or hole-hole effective interaction or to  $E2$  effective charges. Calculations similar to those of Kirson (however using different forces) were recently performed by Jopko and Sprung<sup>65</sup> for the  $fp$ -shell and similar conclusions arrived at. They conclude that the renormalizing effects found in the TDA and particularly the RPA were strongly damped by screening the particle-hole interaction. The results obtained for the screened TDA and RPA are quite similar and intermediate between

those obtained for the  $G_{3p1h}$  correction corresponding to describing the core states as unperturbed particle-hole excitations and the bare TDA. Kuo and Osnes ended up with the same conclusion for effective charge<sup>66</sup> and also for effective interaction<sup>67</sup> for sd- and fp-shell valence nucleons.

Kirson's conclusion-the sum of three series taken together almost vanishes-is depressing since one knows that one does need non-zero renormalization. However, there are two points which offer hope. One is the  $G$  matrix calculations of Barrett et.al.<sup>51</sup> which indicate that the  $G$  matrix can be made much more attractive by varying the intermediate states' spectrum, especially by decreasing the gap between the occupied and unoccupied states. An alternative method for computing  $G$  matrix exactly and simultaneously diagonalizing it for two nucleons outside an inert core was developed by Lawson<sup>68</sup> who solved the coupled integro-differential equation describing such a shell model problem. He also studied the dependence of  $G$  on the gap between the occupied and unoccupied states and obtained results similar to those found by BHM and by McCarthy<sup>69</sup>.

A useful aid in calculating  $V_{eff}$  may be that of shell model diagonalization in a model space of reasonable size (like LoIudice et.al.<sup>70</sup>). Such calculations are very



lengthy and difficult to perform and are probably impossible to carry out for heavy nuclei. But, in cases where such calculations can be performed, they may indicate the correct magnitude of  $V_{\text{eff}}$ . Using these results, one may be able to find a simple expression or model for  $V_{\text{eff}}$ , which can reproduce results similar to those of shell model diagonalization. This method is, in essence, non-perturbative and involves diagonalizing bare  $G$  in an enlarged space. Lo Iudice et.al.<sup>70</sup> performed a shell model calculation of the energy levels of  $A=18$  nuclei in the configuration space of two particles plus three particles and one hole using Kuo  $G$  matrices.

$$\Psi = \sum_{2p} C_{2p} |2p\rangle + \sum_{3p1h} C_{3p1h} |3p1h\rangle$$

These results, when compared with first-order perturbation theory are found to be generally similar. This calculation was repeated by Lo Iudice et.al.<sup>71</sup> however, using a different method of calculation. It turns out that the linked cluster folded expansion converges in  $G$  in a reasonably rapid way. However, the fact that they underestimate the effective charges and  $B(E2)$  values suggests that considerably more core-polarisation is required than they predict it to be. A similar attempt has recently been made<sup>72</sup> for  $A=18$  nuclei by including all

the original Kuo and Brown calculations, namely, the core-polarisation acts like a pairing interaction and depresses in energy the low-lying states of low  $J$ . Barrett and Kirson<sup>9</sup> also calculated  $G_{3p1h}$  and all the large third-order terms contributing to  $V_{\text{eff}}$  with Clement and Baranger<sup>75</sup> matrix elements and the SME and found that the results for the different potentials were similar in that the third-order contributions were large in comparison with the second-order contributions. The results of these calculations would indicate that the convergence problems in trying to compute  $V_{\text{eff}}$  by ordinary perturbation theory (i.e. the relative sizes of terms contributing to  $V_{\text{eff}}$ ) are independent of the form of the N-N potential as long as the potential fits the N-N scattering phase shifts data and bound state properties of the deuteron reasonably well. It was, therefore, also felt that the differences in the off-shell properties of different potentials are not important. Many of the  $G$  matrices which appear in second and higher-order terms are off-the-energy-shell. A study of off-shell effects of this kind has been carried out by Pradhan et.al.<sup>77</sup> who find it is possible for these effects to be quite large—more than 1 MeV for some low-lying states. Again, there is question of the physical validity of the phase shift equivalent  $G$  matrix elements

which produce large off-shell effects<sup>78</sup>. In any case, the influence of off-shell effects on higher-order terms needs to be studied in more detail. Another difficulty concerning calculation of reaction matrix is the choice of the single particle basis e.g. Woods-Saxon wave functions have been used<sup>79,80</sup> for initial and final states between which the matrix elements of  $G$  are calculated and it was found that the  $G$  matrix elements for  $A = 18$  nuclei are appreciably more repulsive for a Woods-Saxon basis than for a harmonic oscillator basis causing upward shifts in the energy spectra by as much as 2 MeV. Yet another difficulty in the calculation of reaction matrix is the proper treatment of the tensor force which is not weak enough and tends to scatter nucleons into intermediate states of medium energy so that the  $G$  matrices which result from potentials which contain the tensor force are still strong. Calculations by Barrett<sup>81</sup> indicate that it is the contribution of the tensor force to the  $G$  matrix which gives rise to the strong collective excitations of the nuclear core and that if the tensor forces are weaker, the contributions of these terms in the perturbation expansion for  $V_{\text{eff}}$  would be less important. Similar conclusions regarding the spectra of  $A=6$  nuclei were arrived at by Lawson<sup>68</sup>.

It should be noted that the calculations by Goode<sup>46</sup> and Kirson<sup>10</sup> do not prove that the perturbation series for  $V_{\text{eff}}$  converges. Their calculations also do not constitute a summation of this series since they do only partial summations. They only show that when certain subsets of diagrams are summed to all orders in  $G$ , one obtains a finite result. One can argue that this procedure, being based on limited physical insight, might overlook important series of terms. Therefore, results of this type, although certainly instructive, can hardly be considered conclusive. Schucan and Weidenmüller<sup>12</sup> have investigated the perturbation expansion for effective operators and algebraically studied its convergence properties. They conclude that, a priori, there is no reason to expect that the perturbation expansion for  $V_{\text{eff}}$  (or any effective operator) converges: it is likely to diverge or at least converge poorly. However, they also show that it is possible to rearrange the series algebraically so that convergence is improved.

Unless a complete absence of many-body forces is established, the next logical step after treating the pair interaction exactly should be treating the three-particle interaction exactly, then the four-particle interaction, and so on - a cluster approach. Such an

approach has had considerable success in the theory of infinite nuclear matter<sup>82,83,84</sup>. Clearly, the convergence of the cluster series will be related to the ratio of the 'interaction volume' of a nucleon to its 'occupation volume' i.e. to the quantity (force range/nucleon separation)<sup>3</sup>. For the short range part  $v_s$ , this is of the order of 10 per cent. Thus, cluster techniques are appropriate for the treatment of  $v_s$  although use of reaction matrix is inevitable. An estimation<sup>85</sup> of three-body forces in nuclear matter suggests that whereas the lowest-order three-body effect is small, second-order effects are larger with the net result of about 2.5 MeV per particle additional binding energy at saturation density. In an analysis<sup>86</sup> of effective interaction in p-shell nuclei, the importance of Feingold's three-body vector interaction<sup>87</sup> arising from second-order effects of the tensor force has been demonstrated. Warke and Gunye<sup>88</sup> have calculated binding energies and r.m.s. radii of nuclei in the mass region  $16 \leq A \leq 208$  in the Jastrow cluster expansion method by including the second-order correction to energy using the Reid soft core N-N potential<sup>89</sup>. They conclude that the contribution of the three-body cluster correction to the two-body correlation energy is at the most 9 per cent. Quesne<sup>90</sup> has generalized the method of Talmi for extracting two-body interactions



from experiment to include all possible many-body forces compatible with the chosen configurations. It is shown that the interactions of the order higher than two are important in  $0f_{7/2}$  shell. Osnes<sup>91</sup> has found that the contributions of effective three-body forces to the binding energies of calcium isotopes calculated with G matrix elements derived from HJ potential are small. Eisenstein and Kirson<sup>92</sup> have shown that if a phenomenological shell model fit to energy levels of  $0f_{7/2}$ -nuclei is performed by using both 'effective' two-body as well as three-body forces, then the contribution due to the effective three-body forces is not negligible. In other words, the microscopic approach invoking core-polarisation renormalization will have to take into account these effective three-body forces as well. Fact is that the problem of nuclear effective interaction is a three-body problem—two valence nucleons and a core. In view of the fact that the ordinary perturbation series for  $V_{\text{eff}}$ , defined in terms of two-nucleon interaction and its renormalization by core excitation, does not converge, Lovas and Vagh<sup>93</sup> have attacked the problem from a three-body point of view. Other calculations<sup>94-96</sup> regarding the size of many-body forces in the three-and more-body problem indicate that they can be significant and hence cannot be neglected. Employing

a procedure first suggested by Brandow<sup>97</sup>, Barrett et.al.<sup>50</sup> constructed the effective interaction in  $A=18$  and  $A=19$  nuclei by performing a direct truncation into a smaller model space using the results of a large shell model calculation. In cases where the truncation is severe i.e. when there is small overlap between the large space and small space wave functions, they find that a large effective three-body term must be added to the effective two-body interaction obtained for  $A=18$  nuclei in order to reproduce the results for  $A=19$  nuclei. On the other hand, the calculations of Quesne<sup>90</sup> indicate that for more than three particles, there is a partial cancellation between the three-body contribution from all other higher-order terms, so that the overall many-body effect is reduced.

Thus, there are many effects which have not been adequately considered or could be treated more accurately in the calculation of  $G$ ,  $V_{\text{eff}}$  and energy denominator and which could possibly lead to reasonable agreement with experiment within the framework of the present theory and available computational techniques. Schucan and Weidenmüller<sup>12</sup> have proposed that the nonconvergence of the perturbation series follows from the fact that we have no control over which experimental results will be best reproduced by the theoretical calculations, for

example, the states produced by  $V_{\text{eff}}$  may not correspond to the lowest experimental states i.e. there may be 'intruder' experimental states among the calculated states. It then follows that we will, probably, be forced to introduce phenomenological and/or experimental information into the microscopic theory to guide the calculations of the effective operators away from the physical effects which are causing the expansion to diverge. This point of view has also been advanced by Harvey and Khanna<sup>98-100</sup>. The introduction of such information is no more a downgrading of the microscopic theory than the introduction of  $G$  in place of  $V$  in order to treat the short range correlations. It is simply a matter of letting nature guide the mathematics so that the mathematics will get to the physical answer in the most economical manner.

Without getting involved in the mathematics, let us see what qualitative features we have learned about renormalization corrections, in particular the core-excitation. Even Bertsch<sup>27</sup>, at the time of introducing the idea of core-polarisation, had demonstrated that the core-polarisation process tends to simulate a pairing force. Although the quadrupole component of the core-polarisation is the most important, the other even

multipoles contribute enough to give the overall force a pairing character. The argument was given originally by Kuo<sup>31</sup>. He considered the diagram (Figure 2.2a) where the particle-hole excited pair is coupled to  $(J'', T'')$ . Each vertex in the figure must be a scalar. Therefore, if the particle and the hole are coupled to  $(J'', T'')$ , then the corresponding tensor component of the effective interaction is picked out. This is because the two valence nucleons can be visualized as interacting via wavy lines (the  $G$  interaction) with a  $(J'', T'')$  coupled particle-hole pair squeezed in between. Thus, for this diagram, the core-polarisation correction from a given  $J'', T''$  behaves as an irreducible tensor force of rank  $J'', T''$ . Kuo<sup>31</sup> has made calculations for nickel isotopes in  $1p_{3/2}$   $0f_{5/2}$   $1p_{1/2}$  model space and finds that the  $J'' = 2, T'' = 0$  component provides the largest contribution. It then means that next to pairing, the most important component of the renormalizing force is the quadrupole-quadrupole interaction between the valence nucleons. Mathematically it means a  $P_2$  force. However, the argument is weakened by the fact that above diagram represents only the direct term in the correction. In fact, one should include the exchange term also as shown in Figure 2.2b. In this diagram, we have only one vertex.

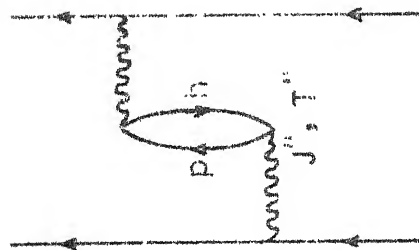


Fig. 2.2a. Direct term of one particle  
-one hole renormalization  
of reaction matrix

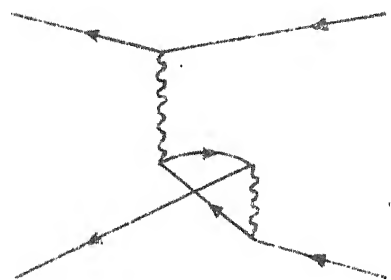


Fig. 2.2b. Exchange term of one particle  
-one hole renormalization of  
reaction matrix

Hence, if the particle and the hole are coupled to  $(J'', T'')$ , then only this component of the force enters the upper interaction but all allowed tensors enter the lower interaction. This means that the  $(J'', T'')$  renormalizing component should not be solely viewed as one of corresponding multipolarity. The correspondence is only approximate.

Freed et.al. have exploited the above arguments. They use Tabakin interaction as residual interaction in lead region thus avoiding handling the singularities. The single particle wave functions in two-particle intermediate states are taken as plane waves. Their contribution is calculated in second Born approximation. However, the core-excitation effects are calculated phenomenologically to simulate the qualitative features discussed above. This approach is thus intermediate between purely phenomenological and purely microscopic approaches. It is argued that the interaction of the valence nucleons through the particle-hole excitations of the core, to some approximation, can be incorporated through a first-order  $P_2$  force. Similarly, discrepancy between calculated and experimental ground state  $0^+$  levels in even-even nuclei may be removed by addition of a pairing force. The procedure for fitting the strength parameters of these renormalizing components

was that first the quadrupole force strength was so adjusted that the first  $2^+$  level was reproduced. Then the pairing force strength was so adjusted that in the presence of quadrupole force of strength as determined above, the ground state  $0^+$  energy is correctly reproduced.

In the present work we take the SME as effective interaction in first order. However, we do not calculate the second-and higher-order corrections microscopically. Instead, like Freed et.al.<sup>101-104</sup>, we have also estimated the renormalization corrections on the basis of qualitative features of the renormalizing force as discussed above. Obviously we have had to introduce both phenomenological and experimental information. However, our attempt has been to use least amount of experimental information. This particular choice of residual interaction greatly conveniences the calculations since the numerical values of relative matrix elements are tabulated<sup>4</sup>. We take the advantage of this in that we can simultaneously perform calculations on several nuclei in different mass regions and thus attempt to explore the properties of effective interaction, say, as a function of mass number. Although the specific choice of SME is purely for convenience, as discussed above, the results are expected to be general and be true for other N-N interactions as well e.g. the

ones with hard core like Yale<sup>105</sup>, HJ etc. or the ones incorporating nonlocality like the one of Tabakin. To avoid ourselves being led into a mess of computational difficulties, we consider nuclei with two valence nucleons only. We hope stopping at two nucleons to be sufficient because we are not considering many-body forces and if only two-body forces are considered, even for a many-valence nucleon system, the interaction energy is a linear sum of two-valence nucleon interactions. However, we consider such nuclei where both  $T = 0$  and  $T = 1$  interactions can be used. Thus, we study the  ${}^6_3\text{Li}$ ,  ${}^{18}_8\text{O}$ ,  ${}^{18}_9\text{F}$ ,  ${}^{42}_{20}\text{Ca}$ ,  ${}^{42}_{21}\text{Sc}$ ,  ${}^{58}_{28}\text{Ni}$  and  ${}^{92}_{40}\text{Zr}$  nuclei. We hope that if we can successfully establish the effective interaction for these nuclei, it will be usable for spectroscopic study of those many-valence nucleons nuclei at least where the valence nucleons are in the same orbit as the lowest active orbit in these nuclei e.g. the  ${}^{19}_9\text{F}$ ,  ${}^{20}_{10}\text{Ne}$ ,  ${}^{93}_{40}\text{Zr}$  nuclei etc. In the present work our emphasis has been only on to see that the two-particle interaction energy in the ground state and the excitation energies of at least a few low-lying levels are reproduced as best as possible although we understand that the task does not finish here. Even if we can arrive at an interaction with which the calculated



level energies agree completely with experiment, this does not guarantee that our wave functions are also good; they might fail to reproduce other properties of levels e.g. transition rates.

## II.2 METHOD OF CALCULATION:

The SME are available as numbers in a form directly usable in nuclear structure calculations. However, the analytical form of the free N-N potential which they represent is unknown and our experience with other known free N-N potentials tells us that it will be complicated enough. We avoid introduction of complicated dependences like explicit dependence on momentum, density etc. Instead let us assume that the interaction is a scalar constructed from combination of spin and orbital degrees of freedom of a nucleon. Since the spin operators are tensors of rank one, we can obtain from  $\vec{\sigma}_1$  and  $\vec{\sigma}_2$  only a scalar ( $\vec{\sigma}_1 \cdot \vec{\sigma}_2$ ), a vector e.g. ( $\vec{\sigma}_1 \times \vec{\sigma}_2$ )<sup>(1)</sup> or a tensor of rank two. Hence, the total interaction is a sum of central, spin-orbit and tensor parts characterized formally by the rank  $k = 0, 1$ , and  $2$  respectively in the scalar product ( $\vec{V}^{(k)} \cdot \vec{S}^{(k)}$ ) where  $\vec{V}^{(k)}$  operates in coordinate space only and  $\vec{S}^{(k)}$  operates in spin space only.

The total interaction is then obtained as

$$V = \sum_k V(k) = \sum_k (\vec{V}(k) \cdot \vec{S}(k)) \quad (2.5)$$

The SME are available as matrix elements of  $V$  between various channels of relative states  $|n^{(2S+1)} \ell_j\rangle$ . However, by employing angular momentum algebra, it is possible to deduce matrix elements of  $V(k)$  from those of  $V$  using

$$\begin{aligned} \langle n' \ell' S j | V(k) | n \ell S j \rangle &= (-)^{\ell+S+j} \begin{Bmatrix} \ell' & S & j \\ S & \ell & k \end{Bmatrix} (2k+1) \cdot \\ &\times \sum_{j'} (-)^{\ell+S+j'} (2j'+1) \begin{Bmatrix} \ell' & S & j' \\ S & \ell & k \end{Bmatrix} \langle n' \ell' S j' | V | n \ell S j' \rangle \end{aligned} \quad (2.6)$$

Further, except for the tensor force channels, the SME are tabulated only for  $n = n'$ ,  $n' + 1$ . However, in a harmonic oscillator basis, other matrix elements with  $(n-n') > 1$  may be obtained from

$$\begin{aligned} \langle n' | V | n \rangle &= \left\{ 2(n'-n-1) \langle n'-1 | V | n \rangle + \sqrt{(n+1)(n+\ell+3/2)} \cdot \right. \\ &\times \langle n'-1 | V | n+1 \rangle + \sqrt{n(n+1+1/2)} \langle n'-1 | V | n-1 \rangle \\ &- \sqrt{(n'-1)(n'-1/2+\ell)} \langle n'-2 | V | n \rangle \\ &\left. + \langle n'-1 | \frac{[r^2, V]}{2b^2} | n \rangle \right\} / \sqrt{n'(n'+\ell+1/2)} \end{aligned} \quad (2.7)$$

The potential is assumed to be momentum independent so that the last term involving commutator of  $r^2$  and  $V$  vanishes.

A complete knowledge of an effective interaction constructed as a sum of various components involves a comprehensive study of the effects of the constituent components on various nuclear properties and on nuclei in various mass regions. If we adopt a totally microscopic approach, given a free two-nucleon interaction, in principle, the effective interaction is obtained as sum of infinite series. For a piecewise study of effective interaction, a properly renormalized free N-N force will be an ideal subject. However, if we want to avoid the use of microscopic approach for calculation of renormalization corrections (as discussed at length earlier in this chapter, the final outcome of a purely microscopic approach indicates its futility) we should have some idea as to the nature of the renormalizations needed. We know, philosophically it is wrong to compare with experiment the results obtained with a free N-N interaction since we know there is a need of renormalizing the force. Nevertheless, a study of the spectra with free N-N force and its central, spin-orbit and tensor components and their comparison among themselves and with experiment

will enable us to draw conclusions about relative importance of these components in nuclear structure calculations and will thus provide us with a clue as to which part needs more attention be paid to and thus guess about the needed renormalizations.

The SME are tabulated as a function of the oscillator length parameter  $b$  ( $= \sqrt{\frac{\hbar}{m\omega}}$ ). Using virial theorem,  $b$  can be related to the r.m.s. radius of the nucleus

$$b = \sqrt{\frac{N \langle r^2 \rangle}{\sum_{nl(\text{occ.})} D_{nl} (2n+2\ell+3/2)}} \quad (2.8)$$

where  $D_{nl}$  is the degeneracy factor i.e. the number of nucleons in an  $(n\ell)$  orbit. Thus, for a completely filled  $(n\ell j)$  orbit,  $D_{nl} = (2j+1)$ . The number  $N$  has to be decided on physical grounds. If  $\langle r^2 \rangle$  is the charge r.m.s. radius,  $N$  will be the total number of protons in the nucleus. If  $\langle r^2 \rangle$  is the matter r.m.s. radius,  $N$  will be the total number of nucleons in the nucleus. The experimental values of r.m.s. radii have been taken from ref. 106..

Once the  $b$  value is fixed, the appropriate relative matrix elements, picked from the tables in ref. 4,

are decomposed into central, spin-orbit and tensor components by employing eq. (2.6).

The required single particle energies are deduced from the spectra of neighbouring odd mass nuclei.

The relative matrix elements are tabulated upto G-wave. However, a study of the numbers reveals that the relative matrix elements decrease rapidly with increasing  $\ell$ . Therefore, we feel it sufficient to include upto  $\ell = 2$  only for calculation of low-lying energy levels.

Harmonic oscillator wave functions have been taken as single particle basis states.

Calculations have been performed with the following interactions:

(i) Full interaction, (ii) central part, (iii) spin-orbit part, (iv) tensor part, (v) central + spin-orbit parts and (vi) central + tensor parts.

The two-body matrix elements in  $jj$ -coupling are calculated using the formula (A.29) given in appendix A.

The respective model spaces for the different nuclei have been chosen within single major shell only. Therefore, only diagonal-in- $n$  matrix elements of  $V$ , except

for the tensor force channel where  $n$  and  $n'$  differ by 1, are needed.

Experimentally, excitation energies of levels are known. To make a comparison with calculated interaction energies feasible, we first calculate the interaction energy in the ground state between the last two particles in a nucleus  ${}^{A+2}_{Z}X$  from known total nuclear binding energies (B.E.) as follows. If both the particles outside the closed shell core are neutrons, the interaction energy is

$$\text{B.E.} ( {}^{A+2}_{Z}X ) + \text{B.E.} ( {}^A_ZX ) - 2 \text{B.E.} ( {}^{A+1}_ZX )$$

and if one is a neutron and the other a proton, the required number is

$$\text{B.E.} ( {}^{A+2}_ZX ) + \text{B.E.} ( {}^A_{Z-1}Y ) - \text{B.E.} ( {}^{A+1}_ZX ) - \text{B.E.} ( {}^{A+1}_{Z-1}Y )$$

In calculating these numbers using these formulae, numerical values of the binding energies are to be taken with a negative sign. The experimental binding energies have been taken from ref. 107.

Below we discuss configuration space, single particle energies and  $b$  values for different nuclei.

i) Op-Shell:

There is ambiguity regarding the value of  $\Delta\epsilon (= \epsilon_{Op_{1/2}} - \epsilon_{Op_{3/2}})$  and the  $b$  value for  ${}^6\text{Li}$  nucleus. The electric charge radius for  ${}^6\text{Li}$  is approximately 2.5 fm. Correspondingly,  $b$ , as defined above, calculates out to 1.84638 fm whereas the value of  $b$  for  ${}^{18}\text{O}$  turns out to be 1.8466 fm. Further, the  $b$  value increases with mass number. As such, it appears that the calculated value 1.84638 fm is too high for a light nucleus like  ${}^6\text{Li}$ . Also, the Stanford data<sup>108</sup> on elastic electron scattering from  ${}^6\text{Li}$  show that the charge form factor for  ${}^6\text{Li}$  could not be interpreted either in terms of the conventional simple harmonic well shell model as used for other p-shell nuclei or in terms of the modified harmonic well shell model in which  $s$  and  $p$  nucleons are assumed to move in different harmonic wells. No acceptable fits to the data could be found from the cluster model approach with either of the two models viz.  $\alpha + d$  and  ${}^3\text{He} + {}^3\text{H}$  structures. However, a fit to the data could be made with the phenomenological expression

for the charge form factor of  ${}^6\text{Li}$  which yields an r.m.s. radius to be  $2.54 \pm 0.5$  fm. If this is so, then harmonic oscillator wave functions are not a suitable complete set that one could have chosen for this nucleus. Instead, one may look for the wave functions generated in some other single particle potential. One calculation<sup>109</sup> yields the r.m.s. radius of  ${}^6\text{Li}$  as 2.52 fm with a parameterized single particle local potential using two different values of the same parameter  $r_0$  of range for the s and p shells.

Lauritsen and Ajzenberg - Selove<sup>110</sup> have not been able to assign an unambiguous value for  $\Delta\epsilon$ . The  $0p_{1/2}$  level in  ${}^5\text{He}$  and  ${}^5\text{Li}$  appears much diffused over a wide energy region. Assimakopoulos et.al.<sup>111</sup> have used a value 5.2 MeV for  $\Delta\epsilon$ . To get over this ambiguity, calculations have been made parameterizing the value of  $\Delta\epsilon$ . Talmi type phenomenological calculations of Cohen and Kurath<sup>112</sup> and Amit and Katz<sup>113</sup> give  $\Delta\epsilon$  to be 0.64 MeV and - 4.74 MeV respectively while Kumar<sup>114</sup> reports a value of around 4 MeV for  $\Delta\epsilon$ . Dawson and Walecka<sup>115</sup>, who calculated the energy levels of  $A=6$  nuclei using the realistic hard core interactions, find that  $\Delta\epsilon \sim 5-6$  MeV gives best agreement with experimental spectrum. Halbert et.al.<sup>116</sup>, however, obtain best fit



for  $\Delta \epsilon = 3.2$  MeV using the HJ potential.

It is possible to prove<sup>117</sup> analytically that the energy splitting between the  $Op_{3/2}$  and  $Op_{1/2}$  single particle levels is given by

$$\Delta \epsilon = \frac{3}{8} \left[ 2V(^3P_0) + 3V(^3P_1) - 5V(^3P_2) \right]$$

where the V's are the diagonal-in-n matrix elements of the potential in the respective relative states. For  $Op$  shell, the energy index  $P (= 2n_1 + l_1 + 2n_2 + l_2)$  is 2. Hence, in relative P - states, only the value zero is allowed for the relative total quantum number n. In Table 2.1 we have tabulated the relevant relative matrix elements for  $b = 1.5$  fm,  $1.6$  fm and  $1.7$  fm.

TABLE 2.1

Diagonal-in-n (=0) SME in relative P-states as relevant to  ${}^6\text{Li}$ .

b \ state (fm)	${}^3P_0$ (MeV)	${}^3P_1$ (MeV)	${}^3P_2$ (MeV)
1.5	- 2.57	3.14	- 1.85
1.6	- 2.46	2.54	- 1.48
1.7	- 2.27	2.08	- 1.18

The value of  $\Delta \epsilon$  turns out to be 5.07 MeV, 3.79 MeV and 2.85 MeV for  $b = 1.5$  fm, 1.6 fm and 1.7 fm respectively. The basic philosophy behind use of realistic interactions is the elimination of free parameters and spectroscopy calculations starting from first principles as far as possible. We see that the SME give the value for  $\Delta \epsilon$  in the range of values just discussed as used by other authors for a  $b$  value in the range 1.5 fm - 1.7 fm. We, therefore, use  $\Delta \epsilon = 3.72$  MeV as used by Joshi<sup>118</sup> and make calculations for three  $b$  values - 1.5 fm, 1.6 fm and 1.7 fm. This way we expect to be able to find the  $b$  value appropriate to this nucleus. However, the energy of ground state  $1^+$  level will depend on the amount of configuration mixing which, in turn, depends on  $\Delta \epsilon$ . Hence, more precisely, the value of  $b$  arrived at would be valid for  $\Delta \epsilon = 3.72$  MeV only.

At the time these calculations were performed only an old compilation<sup>110</sup> of experimental levels of  ${}^6\text{Li}$  was available. They have been compiled again<sup>119</sup> recently. The new energy levels differ little from old values. However, the  $J^\pi$  of second level with  $T = 1$  has been unambiguously established to be  $2^+$ .

ii) 1sOd - shell

For  $^{18}\text{O}$  and  $^{18}\text{F}$  nuclei, the configuration space is

$$\text{Od}_{5/2} \quad 1s_{1/2} \quad \text{Od}_{3/2}$$

For  $^{18}\text{O}$ , we can use single particle levels of  $^{17}\text{O}$ . However, for  $^{18}\text{F}$  it will be more appropriate to take the average of single particle energies in  $^{17}\text{O}$  and  $^{17}\text{F}$  nuclei<sup>120</sup>.

$^{17}\text{O}$	(MeV)	$^{17}\text{F}$	(MeV)
$5/2^+$	0	$5/2^+$	0
$1/2^+$	0.87081	$1/2^+$	0.49533
$3/2^+$	5.08300	$3/2^+$	5.10300

Hence, the single particle energies for the two nuclei are

$^{18}\text{O}$	(MeV)	$^{18}\text{F}$	(MeV)
$\text{Od}_{5/2}$	0	$\text{Od}_{5/2}$	0
$1s_{1/2}$	0.87081	$1s_{1/2}$	0.68307
$\text{Od}_{3/2}$	5.08300	$\text{Od}_{3/2}$	5.09300

The experimental spectra have been taken from ref. 121.

We have used  $b = 1.3$  fm for both  $^{18}\text{O}$  and  $^{18}\text{F}$ .

iii) Of1p - shell

For  $^{42}\text{Sc}$  and  $^{42}\text{Ca}$  nuclei the configuration space is

$$0f_{7/2} \quad 1p_{3/2} \quad 1p_{1/2} \quad 0f_{5/2}$$

The single particle energies in  $^{41}\text{Ca}^{122}$  and  $^{41}\text{Sc}^{123}$  nuclei are

$^{41}\text{Ca}$	(MeV)	$^{41}\text{Sc}$	(MeV)
$7/2^-$	0	$7/2^-$	0
$3/2^-$	2.1	$3/2^-$	1.9
$1/2^-$	3.9	$1/2^-$	4.1
$5/2^-$	6.5	$5/2^-$	6.4

Hence, the required values are

	$^{42}\text{Ca}$ (MeV)	$^{42}\text{Sc}$ (MeV)
$0f_{7/2}$	0	0
$1p_{3/2}$	2.1	2.0
$1p_{1/2}$	3.9	4.0
$0f_{5/2}$	6.5	6.45

The charge r.m.s. radius for  $^{42}\text{Ca}$  is 3.53 fm. Hence,  $b = 2.03795$  fm. We use  $b = 2.0$  fm for both  $^{42}\text{Ca}$  and  $^{42}\text{Sc}$ .

The experimental level spectra have been taken from ref. 124.

For  $^{58}\text{Ni}$  nucleus the configuration space is

$1p_{3/2}$                        $0f_{5/2}$                        $1p_{1/2}$

The single particle energies in  $^{57}\text{Ni}$  are<sup>125</sup>

	(MeV)
$3/2^-$	0
$(5/2)^-$	0.76
$(1/2)^-$	1.08

The identification of  $0f_{5/2}$  and  $1p_{1/2}$  single particle levels is doubtful. However, we use the following values as also used by Joshi<sup>118</sup> and by Jain<sup>126</sup>.

	(MeV)
$1p_{3/2}$	0
$0f_{5/2}$	0.78
$1p_{1/2}$	1.08

The charge r.m.s. radius for  $^{58}\text{Ni}$  is about 3.8 fm and  $b$  turns out to be 2.0523 fm. However, for the whole nucleus we should use matter r.m.s. radius rather than charge r.m.s. radius. In  $^{58}\text{Ni}$  nucleus the proton shells close at  $0f_{7/2}$  level while neutrons fill  $1p_{3/2}$  level. Hence the matter r.m.s. radius is expected to be larger than charge r.m.s. radius. We take  $b = 2.1$  fm for  $^{58}\text{Ni}$ .

The experimental energy levels have been taken from ref. 127.

iv) 2s1d0g - shell

For  $^{92}\text{Zr}$ , active orbits are

$1d_{5/2}$        $2s_{1/2}$        $1d_{3/2}$        $0g_{7/2}$

Joshi<sup>118</sup> excludes the  $0g_{7/2}$  level and assumes the single particle sequence as

	(MeV)
$1d_{5/2}$	0
$2s_{1/2}$	1.22
$1d_{3/2}$	2.07

Table 1

We call it set I. Cohen et.al.<sup>122</sup> have given the single particle energies of neutron levels in  $^{89}_{38}\text{Sr}$  nucleus as

	(MeV)
$1d_{5/2}$	0
$2s_{1/2}$	1.138
$1d_{3/2}$	2.045
$0g_{7/2}$	2.205

If we assume that addition of two protons to  $^{89}\text{Sr}$  does not change the neutron single particle levels,

we can use these values for  $^{91}\text{Zr}$  as well. We call it set II. Cohen<sup>128</sup> has also given the single particle energies for  $^{91}\text{Zr}$  as

	(MeV)
$1d_{5/2}$	0
$2s_{1/2}$	1.55
$1d_{3/2}$	2.70
$0g_{7/2}$	2.70

We call it set III. We make calculations with all the three sets. This study might enable us to comment on the importance of the  $0g_{7/2}$  level for low energy levels by comparing results of set I with those of set II and set III. Furthermore, a relative study of spectra with set II and set III may also reveal the relative importance of the  $1d_{3/2}$  and  $0g_{7/2}$  levels because in set III, these two single particle levels are degenerate. The r.m.s. charge radius for  $^{88}_{38}\text{Sr}$  is about 4.1 fm which corresponds to  $b = 2.1284$  fm. We take  $b = 2.2$  fm for  $^{92}\text{Zr}$ . The experimental energy levels have been taken from ref.129.



### II.3 RESULTS AND DISCUSSION:

We first present the results of calculation with bare SME. Results for  $T = 0$  levels are presented in Figures 2.3 - 2.6 while those for the  $T = 1$  levels are presented in Figures 2.7 - 2.14. Results for  $^{92}\text{Zr}$  nucleus presented in Figure 2.14 are those calculated with set II. The single particle energies for  $^{18}\text{F}$  and  $^{18}\text{O}$  and for  $^{42}\text{Sc}$  and  $^{42}\text{Ca}$  have been taken to be different. This will affect the absolute level positions and the exact amount of configuration mixing and hence nuclear properties calculated with the wave functions so obtained. Apart from this, the general qualitative features of  $T = 1$  spectra of  $^{18}\text{F}$  and  $^{18}\text{O}$  and of  $^{42}\text{Sc}$  and  $^{42}\text{Ca}$  are expected to be, and in fact they are observed to be, similar. Hence, we will discuss  $T=0$  spectra of  $^6\text{Li}$ ,  $^{18}\text{F}$  and  $^{42}\text{Sc}$  and  $T=1$  spectra of  $^{18}\text{O}$ ,  $^{42}\text{Ca}$ ,  $^{58}\text{Ni}$  and  $^{92}\text{Zr}$ .

As expected, the calculated level energies are not in agreement with experiment, maximum discrepancy among lowest few levels being for the ground state. We also conclude the oldest known result - central force gives maximum binding energy. The level energies come almost wholly from the central part and, in fact, in all the cases studied, the ground state calculated with central part alone is in best agreement with experiment

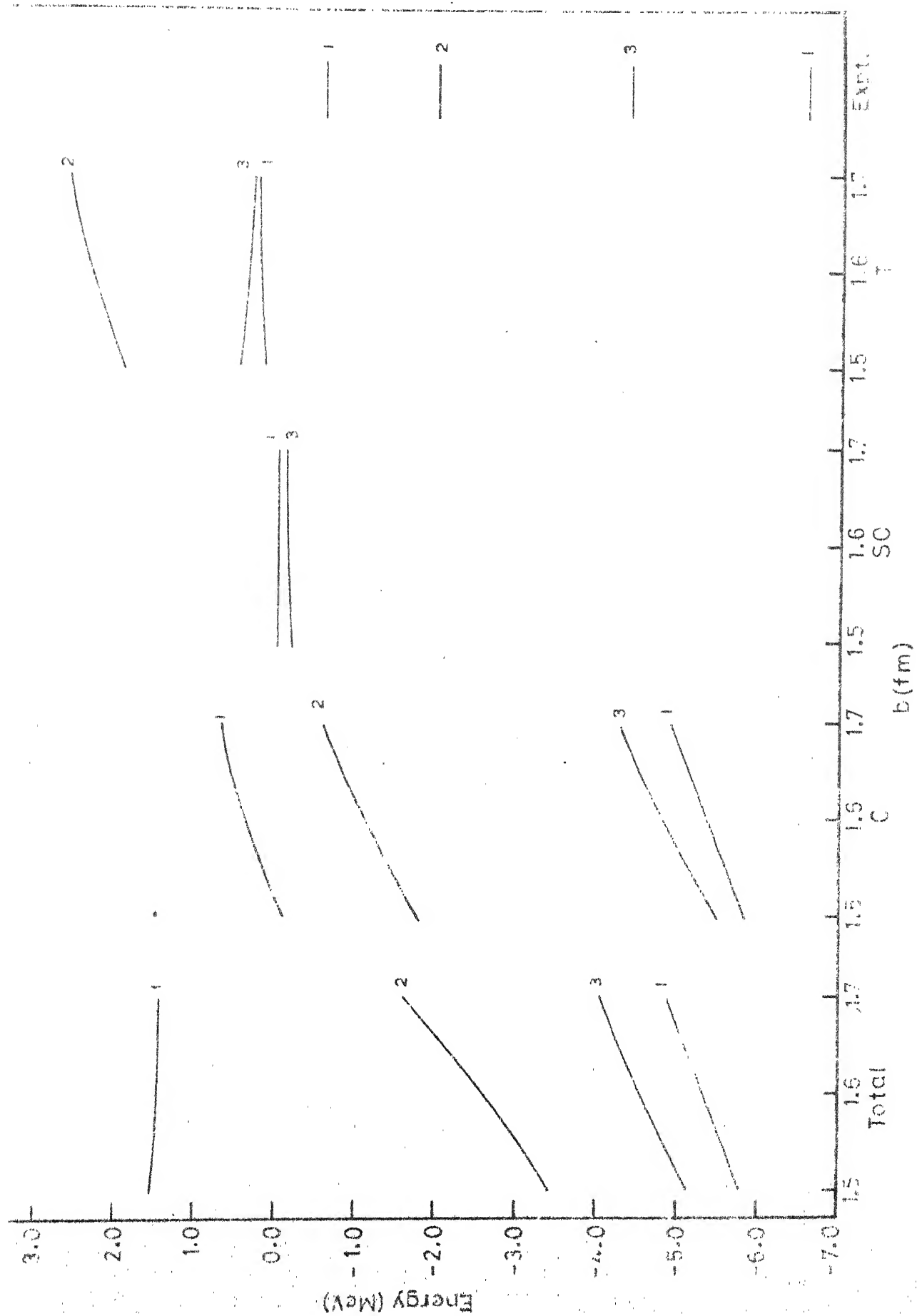


Fig. 2.3

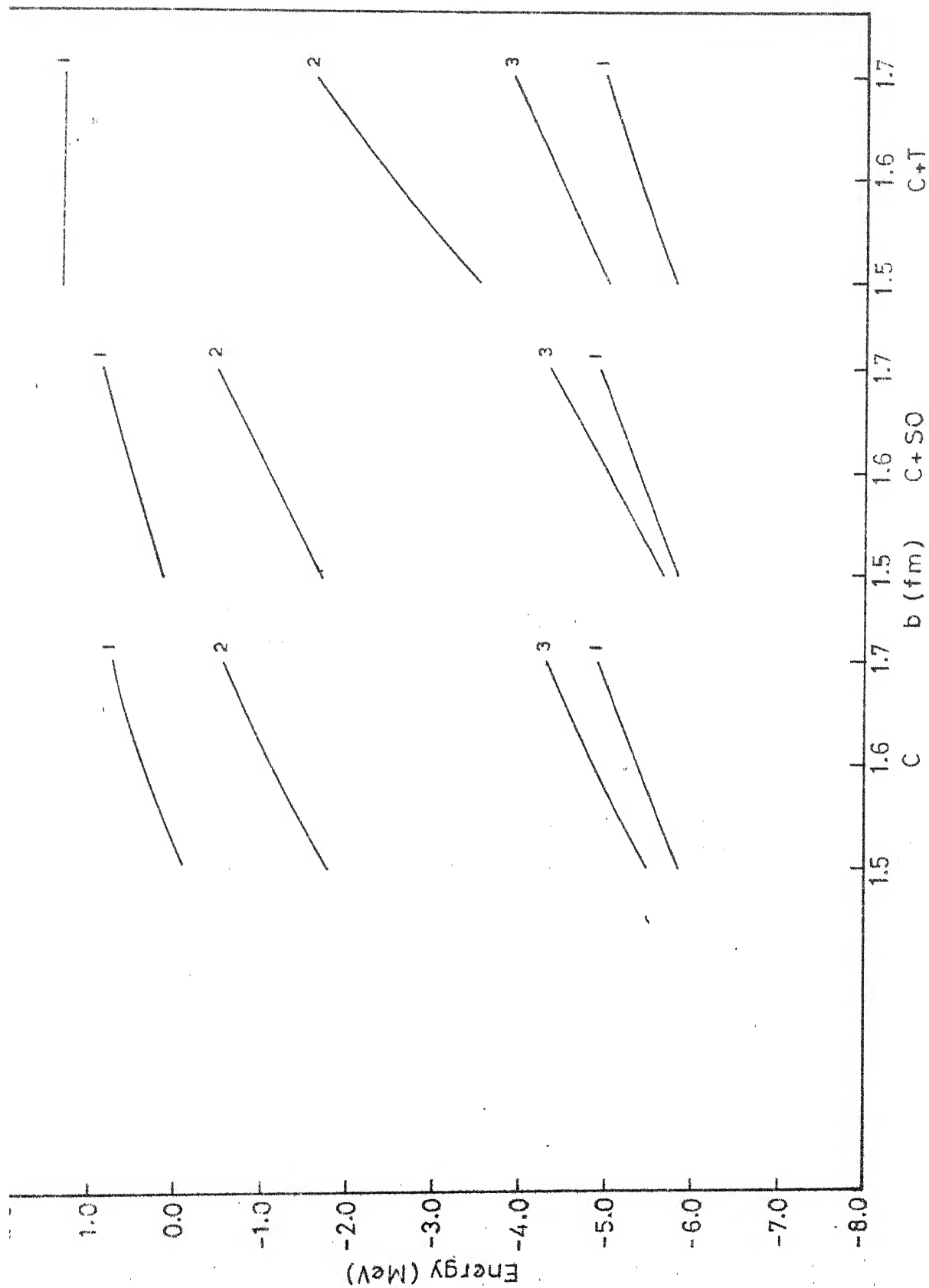
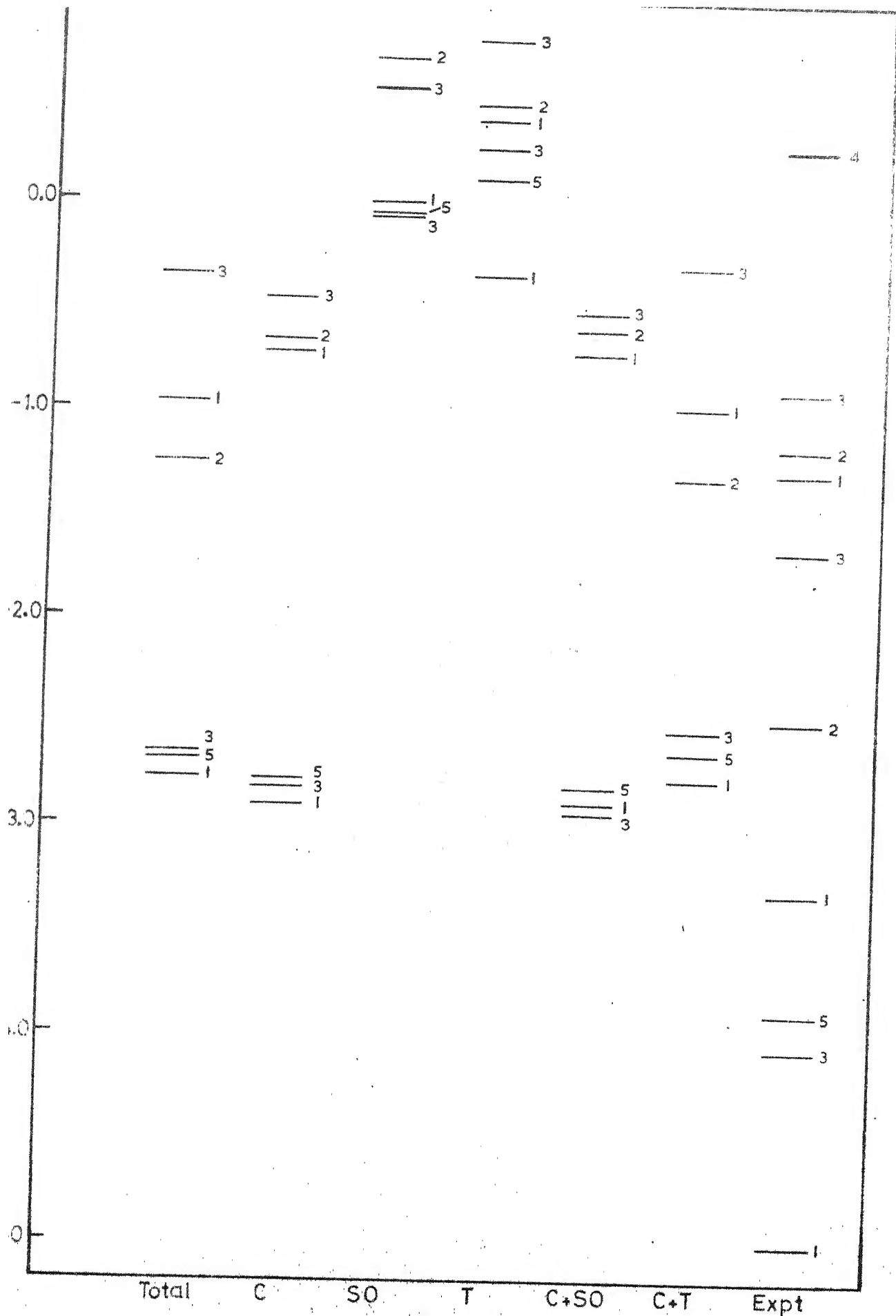


Fig.2.4.



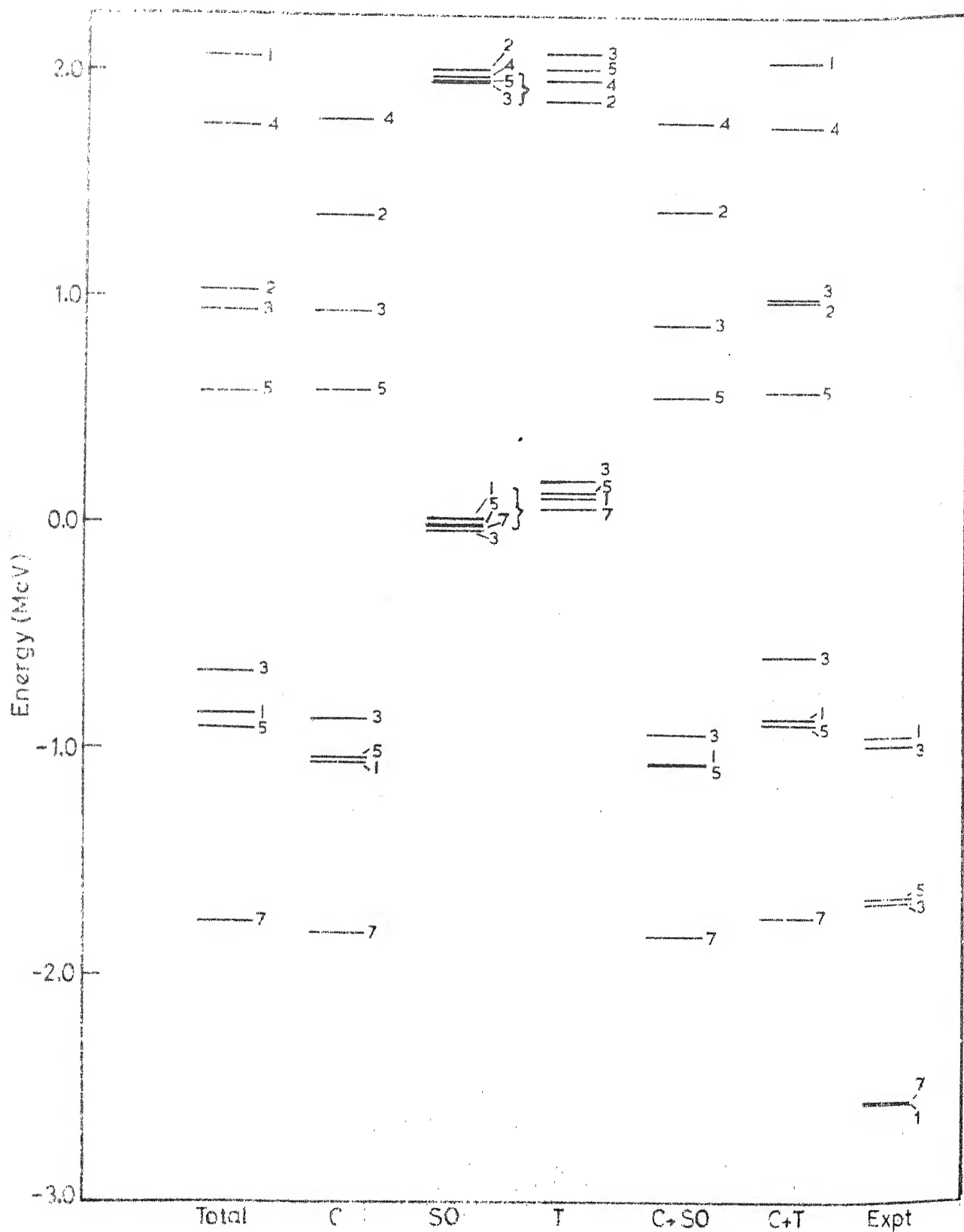


Fig. 12.6. C+O energy levels. Non-experimental.

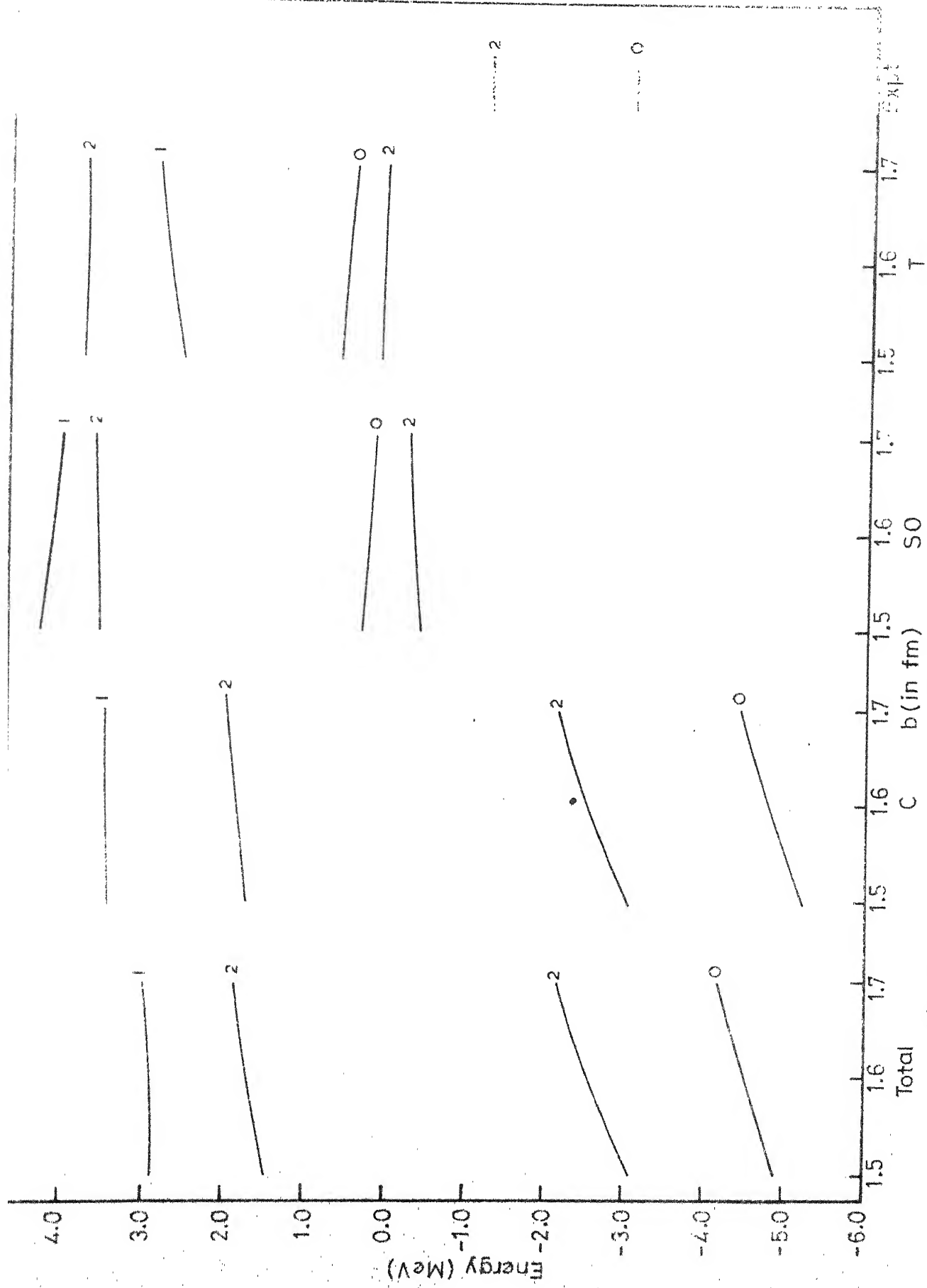


Fig.2.7.  $2 = 1$  spectra of  ${}^6\text{Li}$  plotted as a function of  $b$  values. For explanation of symbols see text.

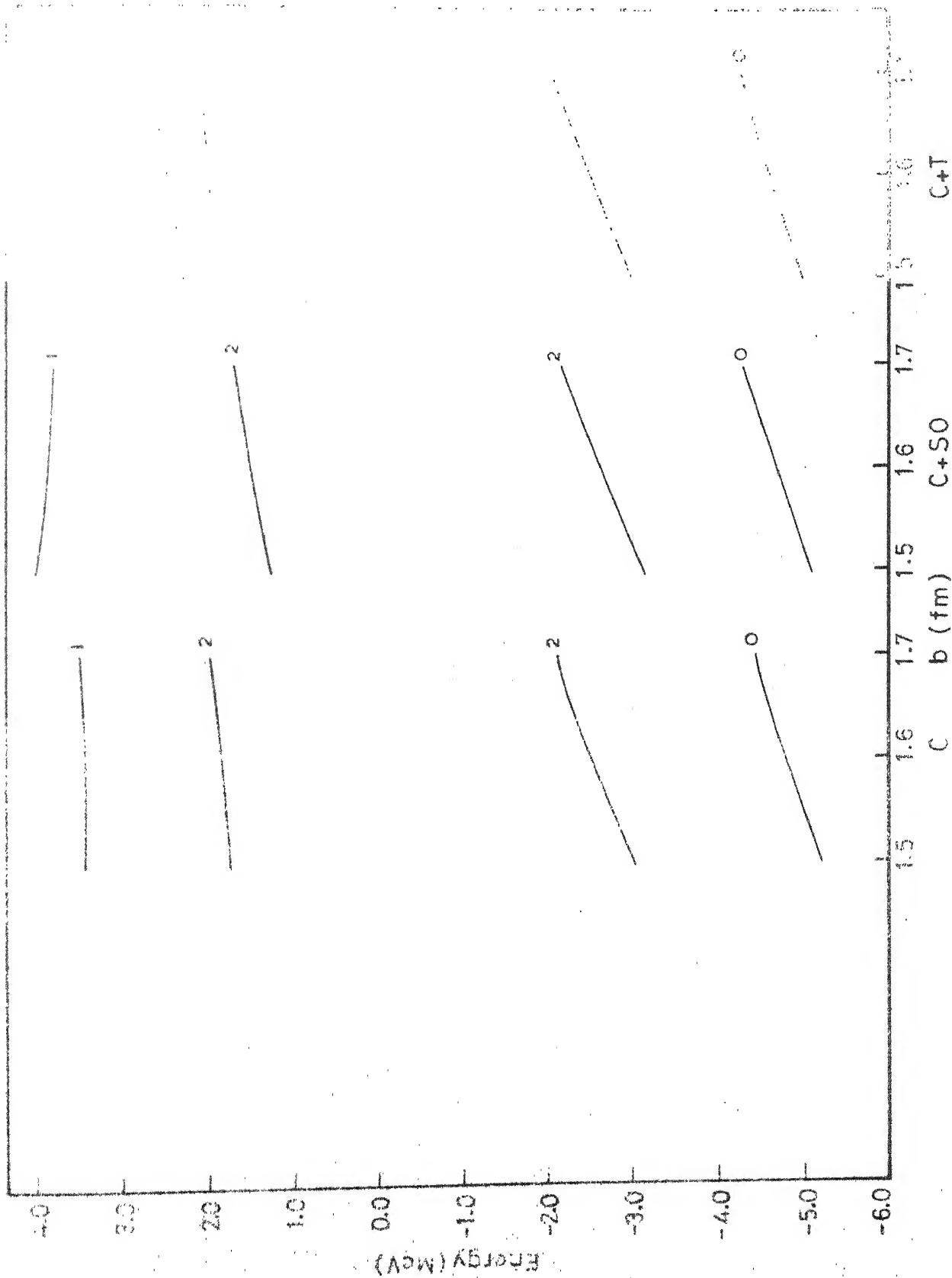


Fig. 1. Energy of  $^6\text{Li}$  plotted as a function of  $b$  value.  
 a) calculation of symbol refer to fig. 2.4.

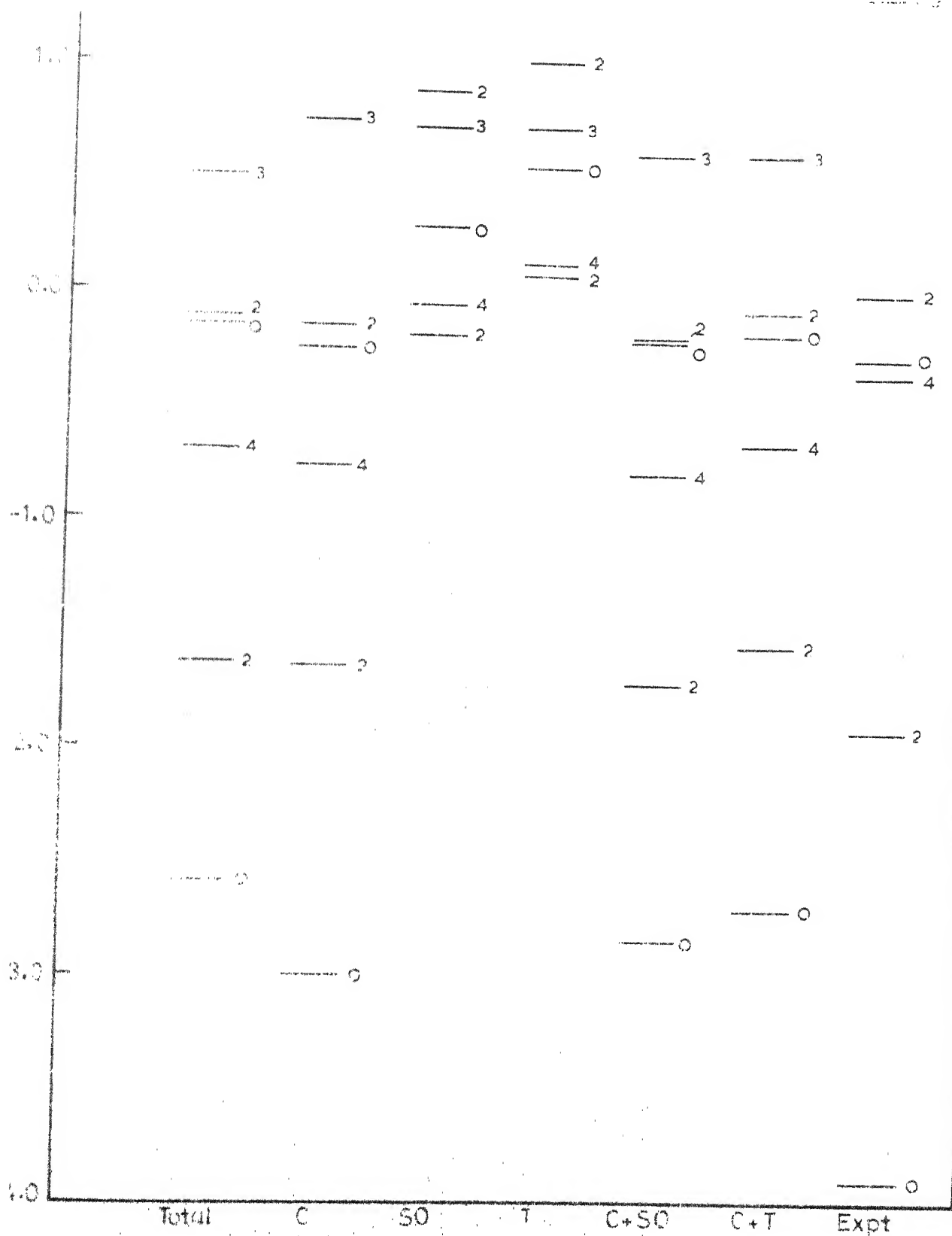


Fig. 1. Difference between experimental and calculated values for various species.



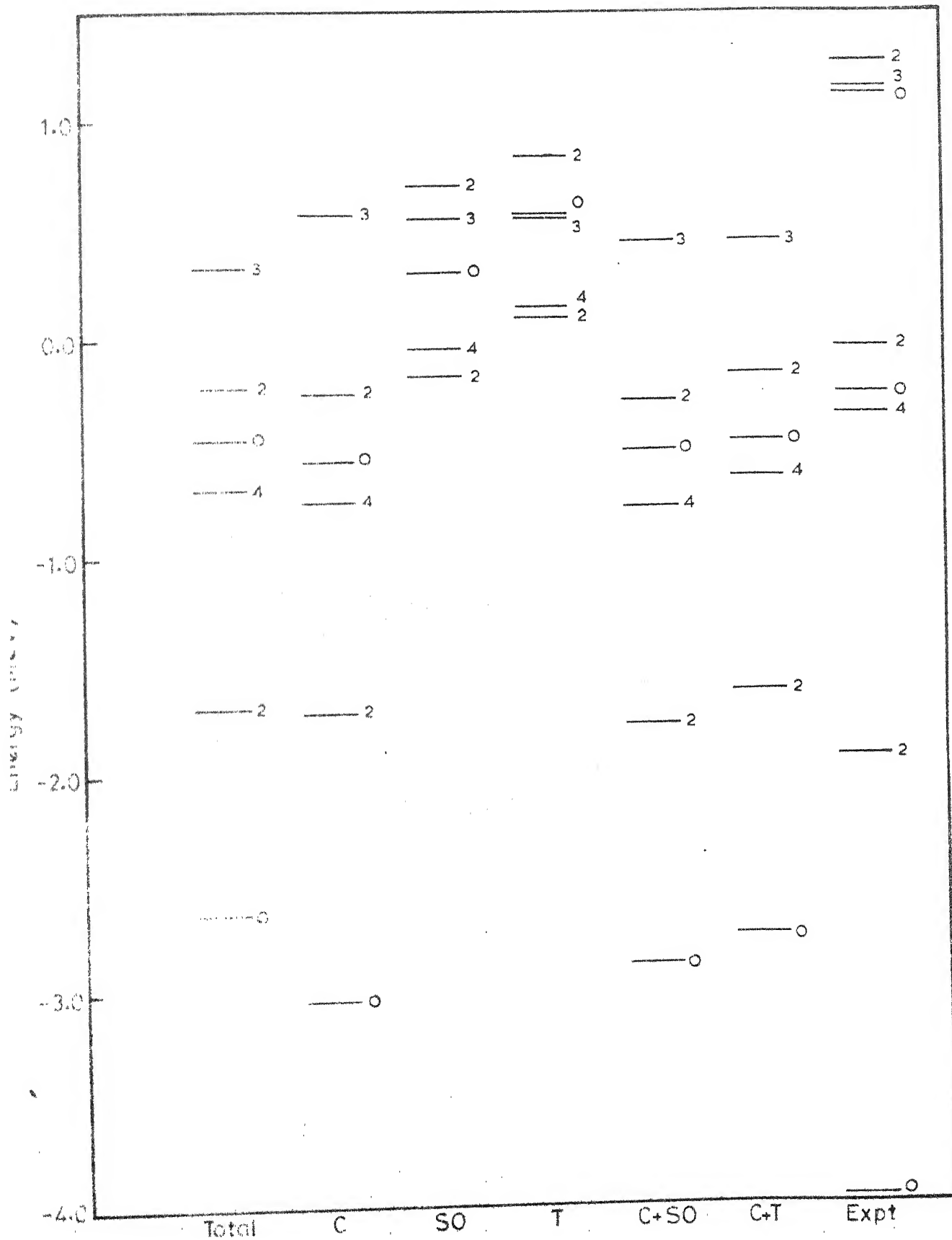
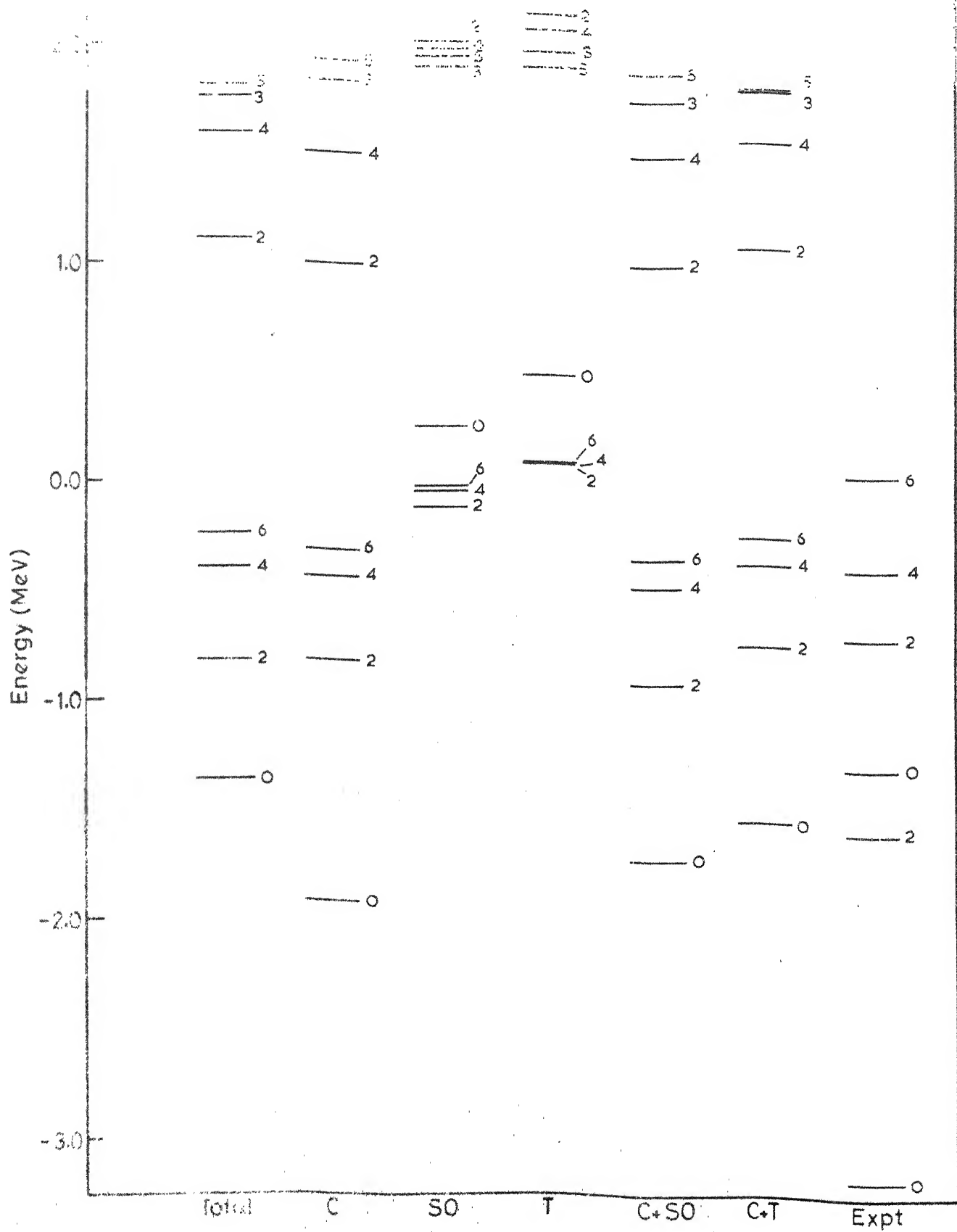


Fig. 2. Net number of  $^{18}O$  not explained by  
simple model of Fig. 1.5.



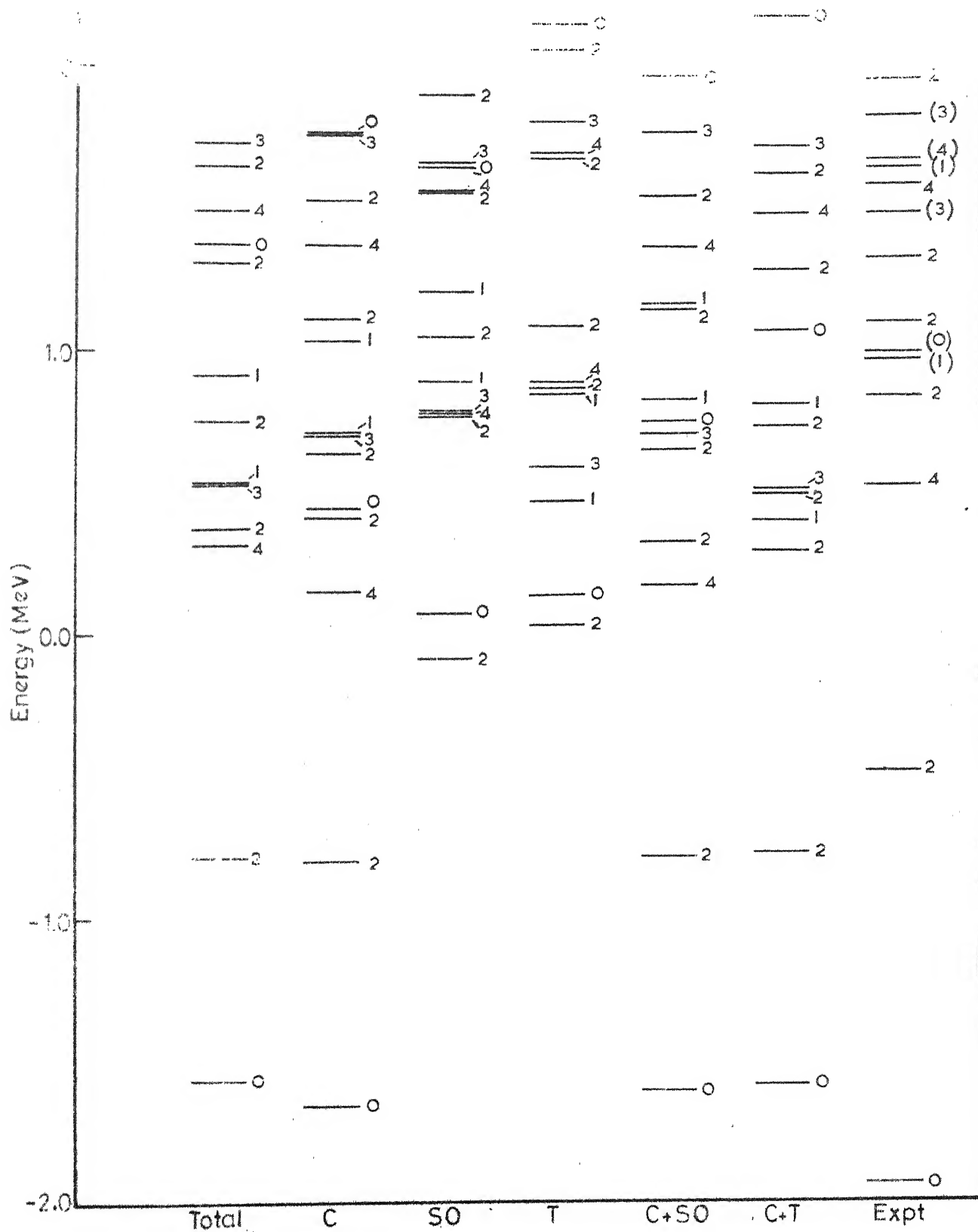


Fig. 2.13 :  $\pi=1$  spectra of  $^{50}\text{Mg}$ . For identification of symbols refer to Figure 2.5.

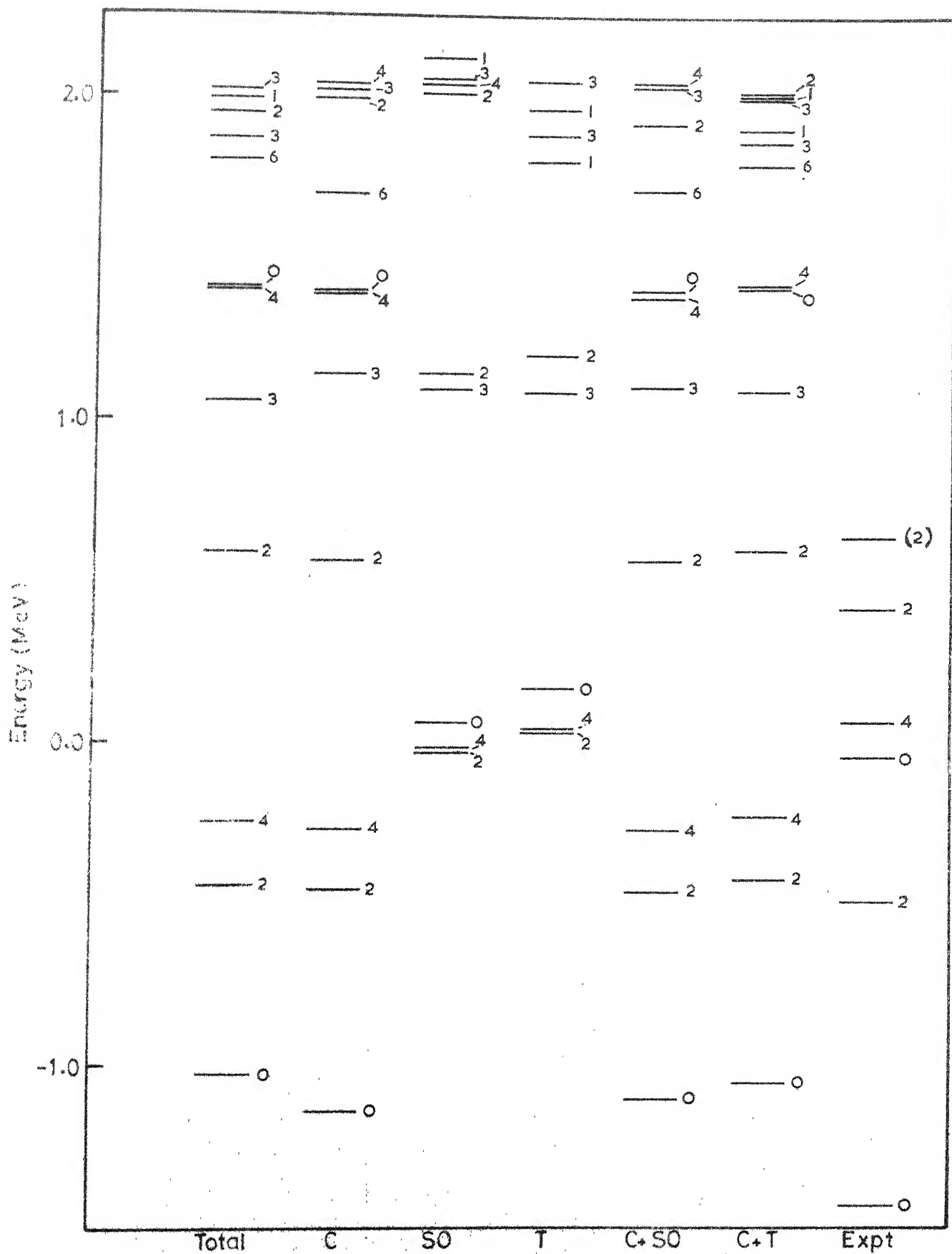


Fig. 2.14: T=1 two-neutron spectra of  $^{92}\text{Zr}$  calculated with set II of single-particle energies. For

and, for ground states, the central part gives larger binding than the total interaction meaning thereby that addition of spin-orbit and tensor parts causes an effective repulsion. It can be verified from the figures that, except for the  $^{18}\text{F}$ ,  $T = 0$  levels, even the lowest state turns out to be unbound when calculated with the tensor part alone.

Besides level energies, the level splittings are also not correctly reproduced, the agreement being worse for  $T = 0$  levels. Let us, for the moment, concentrate only on the levels arising from the lowest  $j^2$  configuration and consider only the total interaction and its central part. Whereas for  $^6\text{Li}$  and  $^{18}\text{F}$  nuclei the calculated spectra are compressed as compared to experimental ones, not only is the ground state  $J^\pi$  of  $^{42}\text{Sc}$  not correctly reproduced but it is also predicted to lie much higher in energy. However, in view of the separation between the bunches of  $(1^+, 7^+)$  and  $(3^+, 5^+)$  experimental levels, the same fact might also be interpreted as predicting that the interaction is too weak to lower down the  $1^+$  level to its right ordered position. Correct ground state  $J^\pi$  of  $^{42}\text{Sc}$  is not achieved with the total interaction, its components or their combinations. The spin-orbit and the tensor parts predict very little

splitting among various J-levels arising from a given two-particle configuration and the calculated levels with these parts are closely bunched near the single particle excitation energy of the two-particle configuration in question. However, the tensor part gives larger splitting than the spin-orbit part. This is in confirmity with the earlier observation<sup>130,131</sup> that the two-body spin-orbit force is mainly exhausted in providing single-particle spin-orbit splittings. From Figure 2.5 one gets an impression that the central part of the  $T = 0$  interaction causes smaller level splitting than does the tensor part and this point is more substantiated when one makes a similar comparison for  $T = 1$  interaction (Figure 2.10) where the observation is not found to be true. However, it can only be called accidental as can be observed from a study of Figure 2.15 where we have plotted the pure  $(0d_{5/2})^2$  levels for the three parts separately. Here we regain the faith that the central part causes much larger splitting than the spin-orbit or the tensor part. The observed bunching is fortuitous and is caused due to the fact that when diagonalization is made, the  $5^+$  level does not change but the  $1^+$  and  $3^+$  levels are pulled down. For the lowest  $j^2$  configuration levels, the splittings due to the spin-orbit and tensor parts are of nearly equal magnitude but the tensor part

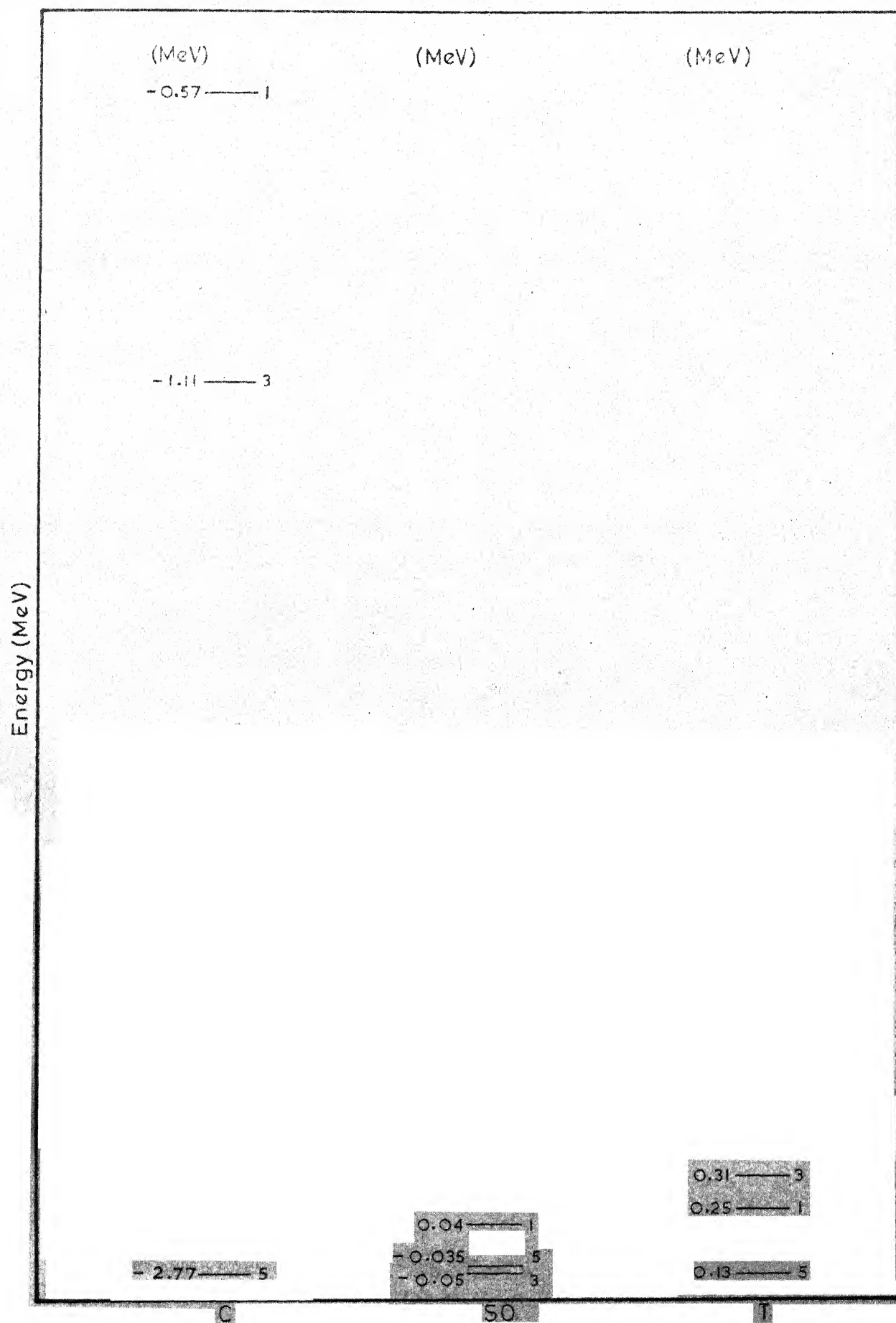


Fig. 2.15

becomes more important for higher energy configurations.

It is observed that the spin-orbit and the tensor parts do not always split a two-particle configuration into different  $J$ 's in the same direction as is done by the central part. Thus, addition of these parts to the central part often results in change in the ordering of the levels. The addition of tensor to the central part results in a drastic increase in the splitting of the  $2_1^+$  and  $1_2^+$  levels of  ${}^6\text{Li}$ . The shuffling of levels as a result of addition of tensor interaction can be seen from spectra of  ${}^{42}\text{Sc}$ . In this case, although the central and tensor parts predict the same level ordering, the ordering of  $1_1^+$  and  $5_1^+$  levels with central + tensor interactions is reversed. The  $3_1^+$  and  $5^+$  levels of  ${}^{18}\text{F}$  are predicted to be reversely ordered with the central part than with the total interaction. However, for lowest few levels, the said shuffling occurs for  $T = 0$  levels only thereby demonstrating the relative importance of the tensor force for  $T = 0$  states. This study is similar to one made by Young<sup>132</sup> who has carried out shell model calculations with purely phenomenological central and central + tensor interactions.

Although the ground state  $J^\pi$  as calculated with tensor part does not agree for  $T = 0$  levels also (except



for  $^{18}\text{F}$ ), the lowest  $0^+$ ,  $T = 1$  level, in all cases, is predicted at a positive energy value well above other levels arising from the lower  $j^2$  configuration. This explains why is it that the difference between the energies of the lowest state, calculated with the total interaction and with the central part respectively, for  $T = 1$  states is much larger than the corresponding difference for  $T = 0$  states. The tensor part appears to be playing an important role for  $^{18}\text{F}$  nucleus. Except for the elevation of the lowest  $0^+$  level, other  $J$  levels of  $T = 1$  from lowest  $j^2$  configuration, calculated with the tensor part, are more closely bunched than the zero isospin levels from the same configuration. This arises because of the fact that we have included the strong off-diagonal tensor force ( ${}^3S_1 - {}^3D_1$ ) that operates in  $T=0$  states only. Otherwise, the tensor components of the pure  ${}^3D_{1,2,3}$  channels of  $T = 0$  and  ${}^3P_{1,2,0}$  channels of  $T = 1$  are much weaker. As calculated, the lowest state in  $^{18}\text{F}$  turns out to be  $0^+$ ,  $T = 1$  with central part;  $3^+$ ,  $T = 0$  with central + spin - orbit parts and  $1^+$ ,  $T = 0$  with central + tensor parts. Thus, presence of tensor interaction is necessary to achieve the correct ground state  $J^\pi$  for this nucleus. The numbers are given in Table 2.2.

TABLE 2.2

Energies and  $J^\pi$  of lowest levels of respective isospins in  $^{18}\text{F}$ , as calculated with various interactions.

Interaction	T = 0		T = 1	
	$J^\pi$	Energy (MeV)	$J^\pi$	Energy (MeV)
Total	$1^+$	-2.76901	$0^+$	-2.64716
Central	$1^+$	-2.90082	$0^+$	-3.04721
Central + spin-orbit	$3^+$	-2.93859	$0^+$	-2.89633
Central + tensor	$1^+$	-2.76922	$0^+$	-2.76369

Overall, it can be said that the agreement for  $T = 1$  levels is better than for  $T = 0$  ones.

A study of eigenvectors obtained with various parts of the force reveals that the central part alone causes appreciable mixing of configurations. Often, there is shuffling of energy levels from ordering that would otherwise be expected from a knowledge of diagonal matrix elements alone. For example, in  $^{18}\text{F}$ , the  $1_1^+$  state lies at  $-1.32$  MeV and comes from  $(1s_{1/2})^2$  configuration. The  $1_2^+$  state lies at  $-0.57$  MeV and comes from  $(0d_{5/2})^2$  configuration. These are the values of diagonal matrix elements. However, after diagonalization, the  $1_1^+$  state shifts to  $-2.9$  MeV energy and is predominantly a  $(0d_{5/2})^2$  configuration (48 per cent contribution) with large admixture of  $(1s_{1/2})^2$  configuration (30 per cent contribution). The  $1_2^+$  state occurring at  $-0.71$  MeV energy receives 68 per cent contribution from  $(1s_{1/2})^2$  configuration and 29 per cent contribution from  $(0d_{5/2})^2$  configuration. The matrix elements of the spin-orbit part are, in general, quite small and the configurations are nearly pure. The tensor part of the interaction alone causes appreciable mixing but less than that due to the central part.

Let us discuss the role of different sets of single particle energies in the  $^{92}\text{Zr}$  nucleus. The results are shown in Figure 2.16. We have plotted only the spectra calculated with the total interaction and with the central part. However, it should be clearly borne that not too serious comparison of the level positions among the three sets should be made since they have been calculated with different sets of single particle energies. However, one thing is clearly seen that the set II gives the best agreement with experimental ground state. The fact that  $O_1^+$  level calculated with set II falls lower than the one calculated with set I can be attributed to various reasons. Let the single particle energies have any value, but inclusion of a new configuration in the configuration space will invariably bring the  $O_1^+$  level down. Even if we had done calculations with set II with  $Og_{7/2}$  configuration chopped off, the calculated ground state would still be expected to be lower than the one with set I since the single particle levels of set II are more closely spaced, and hence more configuration mixing, than those of set I. Similarly, the fact that  $O_1^+$  level with set III lies in between those with set I and set II can be explained on the basis that single particle levels of set III are more

Total

C

— 0

— 0

— 3

— 0

— 0

— 0

— 3

— 0

— 3

— 3

— 3

— 2

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— 0

— 0

— 0

— 0

— 0

— 0

— 0

Set I

Set II

Set III

Set I

Set II

Set III

Expt

widely spaced than those of set I and set II. The relative importance of the single particle levels  $1d_{3/2}$  and  $0g_{7/2}$  can be asserted from a study of the wave functions obtained with set II and set III respectively. In the  $^{92}\text{Zr}$  nucleus, within the model space considered, we expect only four  $0^+$  levels. It turns out that both with set II and set III, when calculated with the central part, the  $0_3^+$  level receives largest contribution from  $(0g_{7/2})^2$  configuration while the  $(1d_{3/2})^2$  configuration constitutes most of the  $0_4^+$  level. This should be viewed together with the fact that in set II the  $0g_{7/2}$  level lies above the  $1d_{3/2}$  level. The actual numbers are given in Table 2.3. This observation can be attributed to the pairing force component of the SME which acts more strongly in states of higher angular momentum. This effect is observed only with the central part of the force and not with the spin-orbit and tensor parts. However, it is acceptable in view of the fact that spin-orbit and tensor forces are comparatively longer range forces whereas pairing force is very short ranged. Similar situation also occurs for total interaction, however, only for set III. First observation means that if only central forces are operative, neutrons prefer to fill the  $0g_{7/2}$  level first -because of the typical pairing force. However, inclusion of spin-orbit and tensor parts

TABLE 2.3

Relative intensities of  $(1d_{3/2})^2$  and  $(0g_{7/2})^2$  configurations in the structure of  $0_3^+$  and  $0_4^+$  levels of  $^{92}\text{Zr}$  as calculated with the total interaction and its central part respectively.

Interaction	Level	Set II		Set III	
		$(1d_{3/2})^2$ (%)	$(0g_{7/2})^2$ (%)	$(1d_{3/2})^2$ (%)	$(0g_{7/2})^2$ (%)
Total	$0_3^+$	95	0.02	1	97
	$0_4^+$	0.01	99	95	2
<hr/>					
Central	$0_3^+$	19	77	8	89
	$0_4^+$	77	21	89	9

weakens the dominating effect of the pairing component to the extent that in presence of all the three components, the neutrons prefer to fill orbits in order of single particle energies. However, if two orbits of different angular momenta but same single particle energy are encountered, the neutrons still prefer to fill the one of higher angular momentum first. This, thus, demonstrates the net dominance of the central part over others.

A study of Table 2.3 reveals that calculations with central part for set II yield more configuration mixing between the  $0_3^+$  and  $0_4^+$  levels even though the  $1d_{3/2}$  and  $0g_{7/2}$  single particle levels are degenerate for set III. It is to be attributed to different values of matrix elements of the potential in the  $(1d_{3/2})_{0^+}^2$  and  $(0g_{7/2})_{0^+}^2$  configurations. The exact numbers for the  $(1d_{3/2})_{0^+}^2$  and  $(0g_{7/2})_{0^+}^2$  configurations are  $-0.17415$  MeV and  $-0.17861$  MeV respectively for the total interaction and  $-0.53563$  MeV and  $-0.99038$  MeV respectively for the central part. The unperturbed matrix elements, including single particle energies, for set II, and set III are shown in Table 2.4. The corresponding perturbed levels are also shown. For central part, the unperturbed  $(0g_{7/2})_{0^+}^2$  level lies lower than the unperturbed  $(1d_{3/2})_{0^+}^2$



TABLE 2.4

Perturbed ( $E$ ) and unperturbed ( $E_0$ ) energies of  $O_3^+$  and  $O_4^+$  levels of  $^{92}\text{Zr}$  calculated with total interaction and its central part.

Interaction		Unperturbed Energies ( $E_0$ )		$E_0(1d_{3/2}^2)$ $-E_0(0g_{7/2}^2)$ (MeV)	Perturbed Energies ( $E$ )		$E(O_4^+)$ $-E(O_3^+)$ (MeV)
		$(1d_{3/2})^2$ (MeV)	$(0g_{7/2})^2$ (MeV)		$O_3^+$ (MeV)	$O_4^+$ (MeV)	
Total	Set II	3.91585	4.23139	-0.31554	4.19182	4.29737	0.10555
	Set III	5.22585	5.22139	0.00446	5.27523	5.45133	0.17610
-----							
Central	Set II	3.55437	3.41962	0.13475	3.38766	3.81607	0.42841
	Set III	4.86437	4.40962	0.45475	4.39721	5.06341	0.66620

level for both set II and set III. As a result of configuration interaction, the  $0_3^+ - 0_4^+$  splitting further spreads up. Something also happens for set III. We may be using any set of single particle energies but the off-diagonal matrix elements, which cause the configurations to mix, always stay the same. The fact that for central part, set II is a case of stronger configuration mixing can now be explained on the basis that the two unperturbed  $0^+$  levels are much closer for set II than for set III. However, calculations with total interaction employing set III yield less mixing than even the calculations with central part and set III even though the splitting between the unperturbed  $0^+$  levels in this case is very small. This may be attributed to the fact that the off-diagonal matrix elements for the total interaction will be different from the ones for the central part. The difference between the matrix elements of total interaction in  $(1d_{3/2})^2_{0^+}$  and  $(0g_{7/2})^2_{0^+}$  configurations is so small that the largeness of single particle energy of the  $0g_{7/2}$  orbit in set II dominates over this difference and the unperturbed  $(0g_{7/2})^2_{0^+}$  level itself lies above the  $(1d_{3/2})^2_{0^+}$  level. Configuration interaction sends them further apart and it turns out to be a case of almost pure configurations. This study also proves that the closeness of two unperturbed levels

is not sufficient to ensure large configuration mixing in wave function. Off-diagonal matrix elements also equally matter. However, for a given set of off-diagonal matrix elements, the closer the unperturbed energies, the stronger is the configuration mixing.

Energy levels of  ${}^6\text{Li}$  calculated with various interactions have been plotted in Figures 2.3, 2.4, 2.7 and 2.8 as a function of  $b$ . It is seen that the spin-orbit part stays almost constant. Largest variations occur in the central part. The tensor part also varies appreciably but in between the central and the spin-orbit variations, however, only for  $T = 0$  interaction. For  $T = 1$  interaction, the variation with  $b$ , of tensor part, is almost as much as that of the spin-orbit part. At any  $b$  value, addition of tensor to central part causes a large depression in  $2^+$ ,  $T = 0$  level and the  $2^+$  level calculated with central + tensor interactions is also the one which varies most sharply with  $b$  value.

We now come to the renormalization part. We have seen that the central force constitutes the major and also the most important component of the two-body force. Therefore, it is anticipated that changes in the matrix elements of this part might bring in the desired

result. In any case, the spectra with pure spin-orbit and tensor forces are nowhere near the truth and it will be a futile attempt to change these parts only. Mathematically, it might be possible to change matrix elements of these forces only and get a new set of matrix elements which could give the right 'numbers' but physically it appears difficult to conceive that these two components in bare interaction have so less importance and the renormalization should change these parts alone. On the other hand, we have other more strong reasons to believe that it might be sufficient to change the central part alone. In any case, it is safe to neglect the spin-orbit part altogether. Spectra with central + spin-orbit and central+tensor interactions respectively are in general resemblance with the spectra with the pure central part both as regards level energies as well as level orderings. However, for finer details, we have seen the importance of the tensor force, particularly for  $T = 0$  interaction. Also, for example, the tensor force, in second-order, has been known<sup>133</sup> to contribute about 150 MeV to  $^{16}\text{O}$  binding energy.

Let us first discuss a possible way of finding a suitable renormalizing force for  $T = 0$  SME. Let it be a  $T = 0$  or a  $T = 1$  state, particularly for ground state, it is expected to be predominantly a relative S-state. For

$T = 0$  it becomes  $^3S_1$  state and for  $T = 1$  it is  $^1S_0$  state. Even experimentally, the largest inaccuracy in determining the matrix elements from scattering data occurs in the  $^3S_1$  state. The coupling parameter  $S$  between the  $^3S_1$  and the  $^3D_1$  channels is also poorly known. This fact makes both  $^3S_1$  and  $^3S_1 - ^3D_1$  matrix elements' values uncertain. However, the tensor force operates in spin triplet states only and, thus, effectively renormalizes the triplet  $S$  - and  $D$  - state central interaction. The relative matrix elements decrease rapidly with  $\ell$ . Neglecting odd state interactions for the moment (which are expected to be much weaker), one might then conclude that the tensor force also effectively renormalizes the  $^3S_1$  state interaction only and that the central part is made almost wholly of the  $^3S_1$  state interaction. It is then expected that if only  $^3S_1$  matrix elements are arbitrarily varied to get a fit with experiment, the net change in these matrix elements will imbibe in itself several effects, namely, the inaccuracy in the bare interaction  $^3S_1$  matrix elements themselves, the renormalization of  $^3S_1$  part itself and the effective renormalization of  $^3S_1$  interaction as a result of possible renormalization of the tensor force in the coupled  $^3S_1 - ^3D_1$  channel.

Therefore, our procedure has been that we make the  ${}^3S_1$  relative state matrix elements  $(1 + \alpha)$  times their bare interaction value and calculate the spectra again with the total interaction so obtained, each time increasing the value of  $\alpha$  and thus pinpoint a value of  $\alpha$  such that a particular level in question is in complete agreement with experiment. There is no a priori reason to believe that a single value of  $\alpha$  will reproduce all the levels. However, if the values of  $\alpha$  as obtained for different levels are not widely different, a least square fit can be attempted to obtain a compromise value of  $\alpha$  such that the considered levels are best, although not exactly, reproduced. We have minimised the function

$$\chi^2 = \sum_i (E_{i,\text{calc}} - E_{i,\text{exp}})^2$$

where the summation over  $i$  runs over the levels considered. The  $E_{i,\text{calc}}$ 's are the level energies calculated as a function of  $\alpha$  and  $E_{i,\text{exp}}$ 's are the corresponding experimental energies.

We now discuss the  $T = 1$  interaction. The  $O^+$  level of  ${}^6\text{Li}$  as calculated with total interaction, for any  $b$  value, is not in agreement with experiment. Similar situation occurs for  ${}^{18}\text{O}$ ,  ${}^{42}\text{Ca}$ ,  ${}^{58}\text{Ni}$  and  ${}^{92}\text{Zr}$  nuclei.

However, there is a difference. In these latter nuclei, the lowest  $O^+$  level occurs as ground state whereas for  ${}^6\text{Li}$  it is an excited state. The calculated  $O_1^+$  level in these nuclei is always above the experimental ground state indicating an insufficient attraction. On the other hand, for  ${}^6\text{Li}$ , the calculated  $O_1^+$  level turns out to be below the experimental one meaning that a repulsive renormalization is needed. As discussed, the  ${}^1S_0$  part of the interaction plays a dominant role for low-lying  $T = 1$  states. In a state where the spins are paired and the relative orbital angular momentum of the particles is zero, the force keeping them in this state is anticipated to be a relatively short ranged one. The exact potential that the SME represent is unknown but with a hard core interaction, the major part of attraction is cut off since it is absorbed in compensating for the hard core. Thus effectively, a hard core realistic interaction is shorter in range than an equivalent well behaved smooth potential, like a phenomenological potential with Gaussian shape. The observation regarding the  $O_1^+$  level suggests that the realistic interaction, let it be SME or others which have been worked upon a number of times, lacks sufficient pairing. If this interpretation is right, it can be checked by adding a pairing force to the bare SME and seeing if it is possible to get correct ground state

energy at least. As a primary calculation we have used a constant strength pairing force defined by

$$\begin{aligned} & \langle j_1 j_2 : J | V_P | j_3 j_4 : J \rangle \\ &= -\frac{1}{2} |G| \sqrt{(2j_1+1)(2j_3+1)} \delta_{J0} \delta_{j_1 j_2} \delta_{j_3 j_4} \quad (2.9) \end{aligned}$$

The results are presented in Table 2.5. These calculations have been done for  $^{18}\text{O}$ ,  $^{42}\text{Ca}$ ,  $^{58}\text{Ni}$  and  $^{92}\text{Zr}$  nuclei only. We see it is possible to get the correct ground

TABLE 2.5

Pairing force strengths  $|G|$  for respective nuclei such that the  $0_1^+$  level energy is correctly reproduced.

Nucleus	$ G $ (MeV)
$^{18}\text{O}$	0.2544
$^{42}\text{Ca}$	0.2480
$^{58}\text{Ni}$	0.0864
$^{92}\text{Zr}$	0.0680



state energy by a suitable choice of the strength  $|G|$ . The valence nucleons in  ${}^6\text{Li}$  are a neutron and a proton and an idealized pairing force as the one defined by eq. (2.9) cannot be used for neutron-proton pairing. For the same reason, these calculations have not been tried for  $T = 1$  states of  ${}^{18}\text{F}$  and  ${}^{42}\text{Sc}$ . For the particular case of  ${}^6\text{Li}$ , the  $0_1^+$  level demands a repulsive renormalization rather than pairing force. In these calculations, the first excited  $0^+$  state cannot be reproduced with the same pairing force strength which reproduces the ground state energy. For excited  $0^+$  levels the calculated energy level varies very slowly as a function of the pairing force strength and if at all we want to reproduce this level too, mathematically it might be possible to get the right number but a physically unacceptable large value of  $|G|$  would be required. This was perceived from the range of values of  $|G|$  during the calculation for obtaining the correct ground state energy and hence was not tried. However, these results are not unexpected either, in view of the fact that the pairing theory is particularly successful for ground states.

Let us again concentrate only on the levels arising from the lowest  $j^2$  configuration. Making a comparison with corresponding energy levels of same  $J^\pi$ ,

one observes that the theory predicts a much compressed spectrum as compared to experiment. Thus, the agreement of energies of  $J \neq 0^+$  levels is better than that of the  $0_1^+$  level. However, it invariably turns out that as a result of compression, the levels of highest  $J$  compatible with the said  $j^2$  configuration (and which also happens to lie highest in energy) always falls below the corresponding experimental level. This means that whereas one invariably needs an attractive renormalizing force to get correct  $0_1^+$  level, one needs an attractive or repulsive renormalization for higher levels, but, as discussed, always a repulsive renormalization for highest  $J$  at least. For example, in  $^{42}\text{Ca}$ , on comparing the results for total interaction with experimental ones, the  $0_1^+$  level is predicted to be too high but the discrepancy is much smaller for  $2_1^+$  level, the  $4_1^+$  level is in excellent agreement with experiment and the  $6_1^+$  level is again in disagreement but below the experimental level. Similarly, the ground state configuration of  $^{58}\text{Ni}$  is  $(1p_{3/2})^2$ . Thus,  $0_1^+$  level is above while  $2_1^+$  level is below the corresponding experimental levels.

One immediate improvement over the pairing force model for the renormalizing force, that has been shown above to be successful for reproduction of correct

ground state energy, is the replacement of the idealized pairing force by a  $\delta$ -function force

$$V = V_0 \delta (\vec{r}_1 - \vec{r}_2) \quad (2.10)$$

The justification for the use of a  $\delta$ -function force is that for the lowest  $0^+$  level it behaves exactly as does the pairing force. However, it also has nonvanishing matrix elements in  $J \neq 0^+$  states and it is, therefore, anticipated that suitable adjustments of strength of the  $\delta$ -function force, when added to the bare SME, might compensate for the renormalizing effects. However, it is well established that the  $\delta$ -function force gives very little splitting in  $J \neq 0^+$  levels while lowering the ground state  $0^+$  level and, therefore, it can be seen beforehand that the strength of  $\delta$ -function force that gives correct ground state energy will not necessarily reproduce the higher levels also. Matrix elements of the  $\delta$ -function potential are calculated using formula (A.28) given in appendix A. The results are presented in Table 2.6. Only results for the lowest  $j^2$  configuration levels are presented and, in fact, these were also the only levels for which some sensible value of  $V_0$  could be found. Otherwise, other excited states were found to vary very slowly with  $V_0$  and for large  $V_0$  they almost

TABLE 2.6

I Nucleus	II J	III Exp. (MeV)	IV Bore (MeV)	V $V_0$ (MeV-fm <sup>3</sup> )	VI (MeV)
<sup>18</sup> O	0	-3.9044	-2.5865	-95.35	-3.90014
	2	-1.9223	-1.6254	-312.50	-1.69464
	4	-0.3515	-0.6887		-0.70959
	0	-0.2727	-0.1402	- 25.55	-0.63336
<sup>42</sup> Cr	0	-3.109	-1.3635	-190.95	-3.10105
	2	-1.589	-0.8172	-504.00	-1.05356
	4	-0.359	-0.3879		-0.52468
	6	0.081	-0.2437		-0.28357
<sup>58</sup> Ni	0	-1.936	-1.5723	-193.80	-1.9383
	2	-0.482	-0.7867		-0.79042
<sup>92</sup> Zr	0	-1.43400	-1.0278	-73.875	-1.43368
	2	-0.49954	-0.441	-85.866	-0.49117
	4	0.061600	-0.2452		-0.25267

became asymptotic to some value. As anticipated, the  $0_1^+$  level is reproducible for all the nuclei. However, not all the levels, even those arising from the lowest  $j^2$  configuration, are reproducible even with different  $V_0$ 's for different levels. In all the four nuclei considered, only those levels, other than the  $0_1^+$  level, were reproducible for which calculated energy was higher than experimental one, and, except for  $^{58}\text{Ni}$ , only the  $2_1^+$  level was found to fall in this category. For others it could have been possible to get the right number by assuming a positive  $V_0$ . However, that would be unphysical. For this reason, the agreement of the said  $2_1^+$  level, when calculated for  $V_0$  that gives correct  $0_1^+$  energy, improves (although exact congruence with  $2_1^+$  experimental level energy is not achieved, since that requires a different  $V_0$  from the one required for the  $0_1^+$  level). The agreement for other levels becomes worse, since, in principle, they require a positive  $V_0$ . Incidentally, the  $0_2^+$  level of  $^{18}\text{O}$  occurring at  $-0.2727$  MeV energy is obtainable for a much weaker  $V_0$  than the one required to get correct  $0_1^+$  level energy. However, the exact shell model configuration of experimental  $0_2^+$  level is uncertain and it has been felt that it contains  $4p - 2h$  deformed component which should be explicitly

included in the model space rather than being treated in perturbation theory. Thus, although we have been able to get the right number, yet, for this reason, we reserve that our wave function for this level may not represent its real structure.

We, thus, see that, to some extent, it is possible to achieve an improved description of level energies by trying to simulate renormalization corrections via a  $\delta$ -function force. If we stop here, we end up with a  $J$ -dependent effective interaction—that too for very few selected levels. The idea of a repulsive  $\delta$ -function force for bound states seems to be more a product of fantasy rather than of any physical meaning. The addition of  $\delta$ -function force only renormalizes the short range part of the  $T = 1$  SME and we would like to attribute the observation, that addition of  $\delta$ -function force only is not sufficient for higher levels which need an effective repulsion, to the fact that the long range part of  $T = 1$  SME also needs be properly renormalized. There is conceptual difficulty in assuming a repulsive  $\delta$ -function force but while constructing a model for long range renormalization we may remember the caution of not introducing a function where such difficulty arises again.

When we calculate the two-body matrix elements (TBME) of  $\delta$ -function potential employing the method of Slater integrals, although all allowed values of  $k$  in the expansion

$$\text{TBME} = \sum_k F^k f_k \quad (2.11)$$

contribute but, finally, owing to the special features of the  $\delta$ -function force and the geometry of expressions occurring in such a way, the TBME is proportional to  $F^0$  only i.e. effectively only  $k = 0$  component contributes. On the other hand, for a non-zero ranged force, all  $k$  values contribute differently, a compact expression involving only one  $F^k$  is not derivable and the relative contributions of different  $k$ 's depend upon the range of force. Roughly, the highest  $k$  value making appreciable contribution varies inversely as the range of the force. Let us, for a moment, make multipole expansion of a finite range Gaussian force

$$e^{-r^2/a^2} = 1 - \frac{r^2}{a^2} + \frac{r^4}{2a^4} \dots \quad (2.12)$$

Let us work in the limit  $a \rightarrow \infty$ . In principle,  $r$  - the two-nucleon separation - also goes to infinity but let us work in a model where wave function fall off for

large internucleon separation

$$r = | \vec{r}_1 - \vec{r}_2 |$$

Defining

$$\vec{R} = \frac{1}{2} ( \vec{r}_1 + \vec{r}_2 )$$

as the centre-of-mass coordinate,

$$r^2 = 2(r_1^2 + r_2^2) - 4 R^2 \quad (2.13)$$

Now, on right of eq. (2.12), first term is a constant and causes no splitting. The second term can be expanded using eq. (2.13). On right of eq. (2.13), first term represents an average oscillator field and the second term represents the motion of the centre-of-mass as a whole. Hence, the second term of eq. (2.12) also does not give any level splitting. The third term can be expanded as

$$\begin{aligned} r^4 = & r_1^4 + r_2^4 + \frac{10}{3} r_1^2 r_2^2 + \frac{8}{3} r_1^2 r_2^2 P_2(\cos \theta) \\ & - 4 r_1 r_2 (r_1^2 + r_2^2) P_1(\cos \theta) \end{aligned}$$

where  $\theta$  is the angle between  $\vec{r}_1$  and  $\vec{r}_2$ .

The first two terms modify the oscillator field. In effect, they introduce anharmonicity. The last term



has odd parity and does not turn out to be valid representation of N-N interaction in physical problems where parity of a two-nucleon state is conserved. Within a major shell, the third term gives the same contribution in all two-particle states. It is the fourth term that has a  $P_2(\cos \theta)$  type angular dependence, conserving parity and which might be expected to produce level splittings.

Therefore, in the long range limit of  $a$ , that the expansion on right side of eq. (2.12) could be terminated at the third term, we see that a long range N-N force, apart from providing the average harmonic oscillator field in which the nucleons move, can be approximately simulated by a dependence of type

$$r_1^2 r_2^2 P_2(\cos \theta)$$

We have derived this particular form for Gaussian shape. However, we expect that, for any general shape of the potential, the angular dependence can be given by  $P_2(\cos \theta)$ . This discussion also explains the fact - the average nuclear field is provided mostly by the long range part of the N-N interaction. Were it not for the largeness of  $a$ , it would not have been possible to terminate the series (2.12) so soon and then the

dependence on  $r_1$  and  $r_2$  of angle-independent terms would be much more complicated.

Thus, in general, we anticipate that a long range force can be approximately represented by

$$f(r_1, r_2) P_2(\cos \theta)$$

where  $f(r_1, r_2)$  is some radial dependence. However, it is customary to take

$$f(r_1, r_2) = r_1^2 r_2^2$$

In this approximation, calculations become extremely simple. The justification for such a simple choice is that if the potential

$$v = \chi r_1^2 r_2^2 P_2(\cos \theta)$$

is included as a part of two-nucleon potential, it generates the deformed field needed to explain quadrupole deformation of deformed nuclei.

The pairing-plus-quadrupole approach has been used<sup>134</sup> extensively in nuclear structure calculations. In these calculations, this sum is taken as the total

residual interaction. However, in our calculations, we are only taking it as the renormalizing force, the pairing and the quadrupole parts renormalizing the short and the long range parts of the free N-N force respectively. For the pairing part we have used  $\delta$ -function force instead of the idealized constant strength pairing force. The choice of pairing and quadrupole forces has been for convenience and also due to our knowledge that these forces have earlier been successfully used. Otherwise, if the philosophy is only to add a short and a long range part whose strength parameters are to be determined from a fit to experimental data, in principle, any phenomenological form for these parts should work. Also, such an approach would be expected to be more successful if the pairing-plus-quadrupole approach is not very successful for many excited levels. This is anticipated because the short range part will largely renormalize the higher  $k$  components of the free interaction while the long range part will mainly contribute to low  $k$  components. That way, a combination of them would give a complete multipole expansion of the renormalizing force. However, it has not been tried since calculations are anticipated to be more involved and if several strength and range parameters are included, that would spoil our case of formulating an effective

interaction in whose derivation a minimum number of experimental levels are used. For this reason we have restricted upto pairing and quadrupole forces only.

Although we have given a different explanation for use of quadrupole force as a component of renormalizing force, we could have anticipated at least for the angular dependence to be of the type  $P_2(\cos \theta)$  from an analysis of second-order perturbation theory results as done earlier in this chapter.

Matrix elements of the quadrupole force are calculated using eq. (A.24) as given in appendix A. However, it can be seen that inclusion of this new renormalizing force increases the number of unknown parameters to three (the  $\delta$ -function force strength and the quadrupole force strengths in spin-singlet and triplet states respectively) from one and thus the basic point, that the theory should contain no or minimum number of parameters, behind the use of realistic interactions seems to be losing, since, like this, we can go on adding physically acceptable renormalizing forces one after the another and then one can question the use of such a method at all - compared to such a procedure, the use of a completely phenomenological force will also be equally justified. To avoid this objection, we

adopt a procedure wherein we effectively use only one experimental level for determination of the three parameters, although the computer time is increased in this process. We use only the ground state energy for determination of the parameters. First a rough guess of the upper limit of parameters is obtained in such a way that, other two parameters remaining zero, the two-body matrix element for  $0_1^+$  level itself becomes equal to the experimental level energy. This is the upper limit value for this parameter since even at this value, as the configuration mixing calculation is done, the calculated ground state will certainly move below its unperturbed value (i.e. the experimental value) and therefore, if, starting from zero, the strength for this particular parameter is increased in small steps, even if the other two parameters do not contribute at all, we will be able to pin-point a value where the calculated ground state energy, with this parameter only nonvanishing, agrees with the experimental ground state energy.

In any case, the  $\delta$ -function force has to be kept attractive but the quadrupole force strength can be taken to be attractive or repulsive. In fact, when all the three parameters are simultaneously varied, there can be a number of sets of values that give the same description

of the ground state energy. Now, it is here that, if required, we can take one or both spin components of the quadrupole force to be repulsive. The quadrupole force does contribute in  $0^+$  states also. Hence, introduction of a repulsive component in the effective force requires the attractive part to be stronger in order to get correct ground state energy. Now, the  $\delta$ -function force contributes to  $J \neq 0^+$  states also. Therefore, eventually, a limit to the variation of parameters is set, both on positive and negative side beyond which agreement of higher levels cannot further improve.

After pin-pointing parameter values for ground state energy, excited states are calculated with each set. It then turns out that not all the sets can describe the excited states equally well. It would be desirable that a single set of parameters describes all the excited states. However, if it is not possible, we can, at least, find a set, different for different levels, that gives best agreement for one level at a time. Thus, effectively we will end up with a  $J$ -dependent effective interaction.

Since the  $T = 1$  levels of  ${}^6\text{Li}$  require a repulsive renormalization, we cannot use a  $\delta$ -function force.

experimental levels as compared with results for  $b = 1.5\text{fm}$  and  $1.6\text{ fm}$  but the  $1_1^+$  level is in worst agreement which means that a comparatively much larger renormalization is needed for the  $1_1^+$  level. The results are tabulated in Table 2.7 and plotted in Figure 2.17.

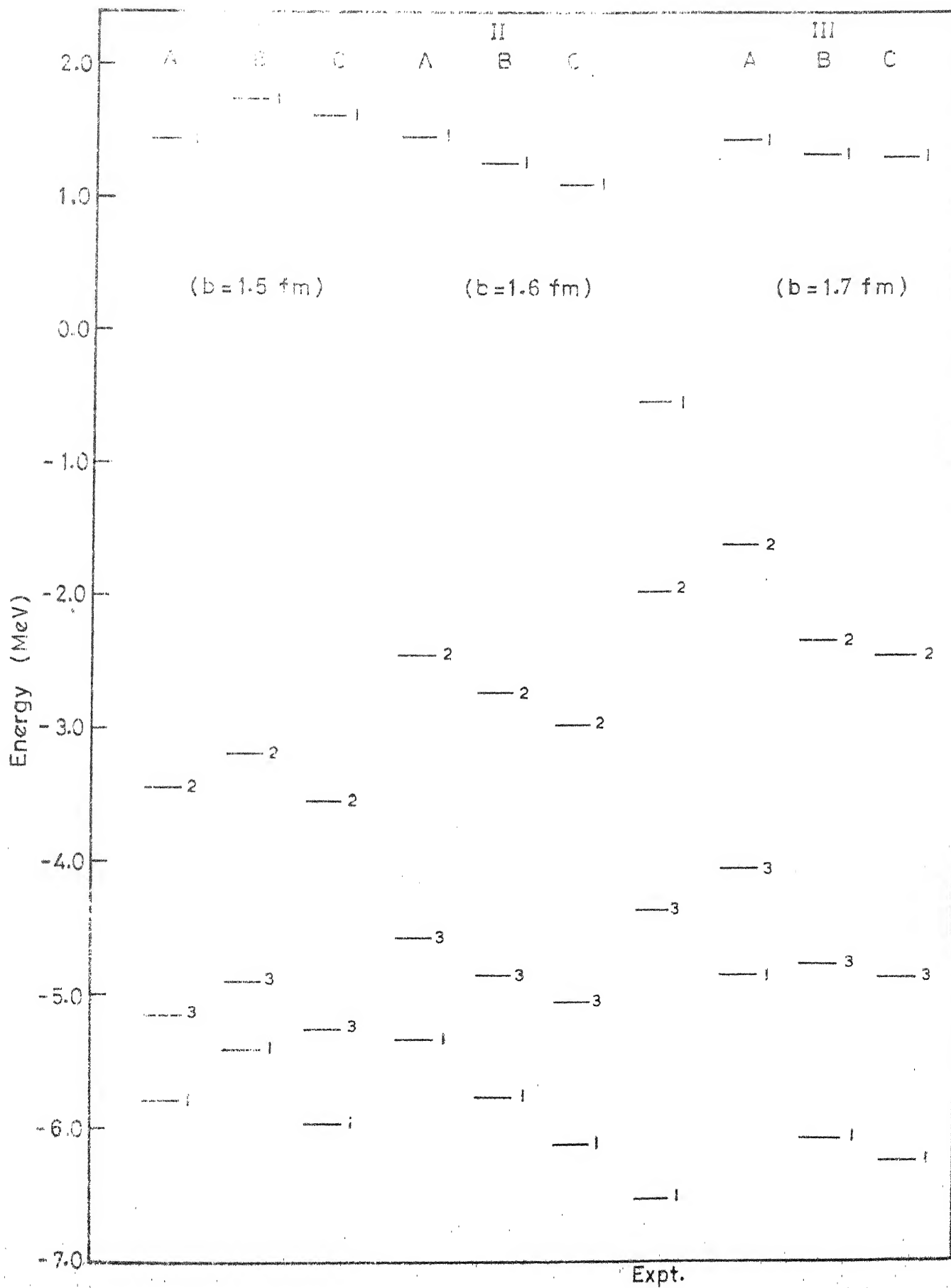
One thing can be observed - except for  $b = 1.7\text{fm}$ , for  $b = 1.5\text{ fm}$  and  $1.6\text{ fm}$ , the value of  $\alpha$  for the  $2^+$  level is almost twice that for the  $3^+$  level. It may also be noted that the  $2^+$  level comes from the  $(0p_{1/2} 0p_{3/2})$  configuration while the  $3^+$  level comes from the ground state configuration  $(0p_{3/2})^2$ . We have earlier made a mention that the low-lying states are predominantly relative S-states. This observation makes us suspect that may be for the  $2^+$  level, effects of higher partial waves cannot be entirely simulated in the  $^3S_1$  matrix elements and that may be this approach for renormalization is more successful only for levels arising from the lowest  $j^2$  configuration. Even otherwise, we know that a good  $\chi^2$  fitting is possible only if the numbers to be fitted are not very much different from one another. Therefore, we have repeated the calculations for  $\chi^2$  fitting without including the  $2^+$  level. Largest change in  $\chi^2$  from this omission occurs for  $b = 1.5\text{ fm}$  where the best fit value of  $\alpha$  becomes positive after

$b$ (fm)	S. No.	$1_1^+$	$2^+$	$3^+$	$1_2^+$	
		Exp. (MeV)				
	1	Bare (MeV)	-5.79861	-3.445	-5.16	1.53477
	2	$\alpha$	0.0980958	-0.29348	-0.15888	
	3	$\alpha_0$		-0.049981		
	4	Best fit (MeV) (with $\alpha_0$ )	-5.4149	-3.19583	-4.91083	1.73881
1.5	5	$\chi^2$ (MeV) <sup>2</sup>		3.06077		
	6	$\alpha'_0$		0.021979		
	7	Best fit (MeV) (with $\alpha'_0$ )	-5.96734	-3.55457	-5.26957	1.6245
	8	$\chi^2$ (MeV) <sup>2</sup>		1.15465		



1	Bare (MeV)	-5.34523	-2.46	-4.58	1.45669
2	$\alpha$	0.16828624	-0.10607	-0.04764	
3	$\alpha_0$			0.06709	
4	Best fit (MeV) (with $\alpha_0$ )	-5.78769	-2.73461	-4.85461	1.25149
5	$\chi^2$ (MeV)			1.38738	
6	$\alpha'_0$			0.10831	
7	Best fit (MeV) (with $\alpha'_0$ )	-6.12184	-2.94198	-5.06198	1.09654
8	$\chi^2$ (MeV) <sup>2</sup>			0.61521	

1	Bare (MeV)	-4.86631	-1.63	-4.06	1.44235
2	$\alpha$	0.2543166	0.09889	0.07778	
3	$\alpha_0$			0.18318	
4	Best fit (MeV) (with $\alpha_0$ )	-6.0801	-2.35542	-4.78542	1.32113
5	$\chi^2_{(\text{MeV})^2}$			0.53636	
6	$\alpha'_0$			0.208	
7	Best fit (MeV) (with $\alpha'_0$ )	-6.24481	-2.45384	-4.88384	1.30469
8	$\chi^2_{(\text{MeV})}$			0.360457	



the omission. This should be viewed together with the fact that, with  $2^+$  level included in the fit, the  $1_1^+$  ground state renormalized level is in even worse agreement with experimental level than what agreement the bare interaction itself can give. Omission of the  $2^+$  level from fit causes the agreement to improve on renormalization. At all the three  $b$  values,  $\chi^2$  improves when the  $2^+$  level is not included in the fit. drastic improvement occurs for  $b = 1.5$  fm. For  $b = 1.7$  fm, the  $2^+$  level calculated with bare interaction is not very much different from experimental level and also the value of  $\alpha$  for this level at this  $b$  value is positive. Hence, improvement in  $\chi^2$  for  $b = 1.7$  fm is not as much as it is for  $b = 1.5$  fm.

The  $1_2^+$  level is also explained better after modification of the  $^3S_1$  matrix elements. However, it varies very slowly with  $\alpha$  and it could be perceived that a very large value of  $\alpha$  would be required if at all this level does not asymptotically approach a constant value as was also the indication during the range of  $\alpha$  values considered. This has been the criterion throughout that calculation of  $\alpha$  for all those levels was not tried for which it could be observed that a physically inconceivably large value of  $\alpha$  would be required. We can only reason that it is not justified to assume that the renormalization

of the force in various channels can be effectively dumped into the matrix elements of the  ${}^3S_1$  relative state alone for all the states of a nucleus.

The spectrum of  ${}^6\text{Li}$  is best reproduced for  $b = 1.7$  fm. However, it does not necessarily mean that it is also the true  $b$  value for this nucleus. At the most we can say that, consistent with  $\epsilon_{\text{Op}_{1/2}} - \epsilon_{\text{Op}_{3/2}} = 3.72\text{MeV}$ ,  $b = 1.7$  fm is the most reasonable value of  $b$  for this nucleus. We have not made calculations for some still higher value of  $b$ , say  $b = 1.8$  fm, but it can be seen from the figures that if the levels continue to behave with  $b$  in the same regular fashion (which is expected also in view of the fact that the relative matrix elements vary smoothly with  $b$ ), the agreement of levels calculated with bare interaction will become worse (particularly for the ground state) although it might be possible to arrive at a more satisfactory best fit value of  $\alpha$ . We suppose this ambiguity will continue to prevail unless the  $b$  value and the single particle energy of the  $\text{Op}_{1/2}$  level is uniquely established.

One can reasonably question that if three known values are different, a one-parameter fit to two of them is bound to be better than the fit to all of them. It would then weaken our possible conclusion, that a

reasonable renormalization can be established in terms of  ${}^3S_1$  matrix elements alone, particularly for the levels arising from the lowest  $j^2$  configuration, which appears to be emerging by the observation of a better fit to  $1^+$  and  $3^+$  levels of  ${}^6\text{Li}$  on exclusion of the  $2^+$  level.

This doubt can be checked by performing similar calculations on  ${}^{18}\text{F}$  and  ${}^{42}\text{Sc}$  nuclei - the  $(\text{Od}_{5/2})^2$  and  $(\text{Of}_{7/2})^2$  configurations give respectively three and four levels. The results for  ${}^{18}\text{F}$  are tabulated in Table 2.8 and plotted in Figure 2.18. Similarly, numbers for  ${}^{42}\text{Sc}$  are shown in Table 2.9 and these are plotted in Figure 2.19. It is seen that the agreement does improve a lot when only levels from the lowest  $j^2$  configuration are considered in the fitting procedure even though it is also possible to find out reasonable values of  $\alpha$  for one or two other levels as well. The value of  $\alpha$  for the  $4^+$  level of  ${}^{18}\text{F}$  differs much from the  $\alpha$  values for  $1^+$ ,  $3^+$ ,  $2^+$  and  $5^+$  levels and therefore,  $\chi^2$  is very much improved when  $4^+$  level is excluded from the fit. The  $\chi^2$  improves further when the  $2^+$  level is also excluded from the fit. However, this time the change in the value of  $\chi^2$  is not substantial. Similar results are found in case of  ${}^{42}\text{Sc}$  nucleus also.

TABLE 2.8

S.No.	$1^+$	$2^+$	$3^+$	$4^+$	$5^+$
	EXP (MeV)	-2.4843	-4.0713	0.2923	-3.8865
1	Bare (MeV)	-2.769	-2.6527	1.9672	-2.6870
2	$\alpha$	0.450	0.44875	0.635	0.4585
3	$\alpha_0$		0.47022		
4	Best fit (MeV) (with $\alpha_0$ )	-5.1201	-4.1526	0.7258	-3.9214
5	$\chi^2_{(\text{MeV})^2}$		0.21526		
6	$\alpha'_0$		0.44730		
7	Best fit (MeV) (with $\alpha'_0$ )	-5.0055	-4.0795	0.78637	-3.8609
8	$\chi^2_{(\text{MeV})^2}$		0.00112		
9	$\alpha''_0$		0.44862		
10	Best fit (MeV) (with $\alpha''_0$ )	-5.0121	-4.08370	0.78277	-3.8643
11	$\chi^2_{(\text{MeV})^2}$		0.000658		

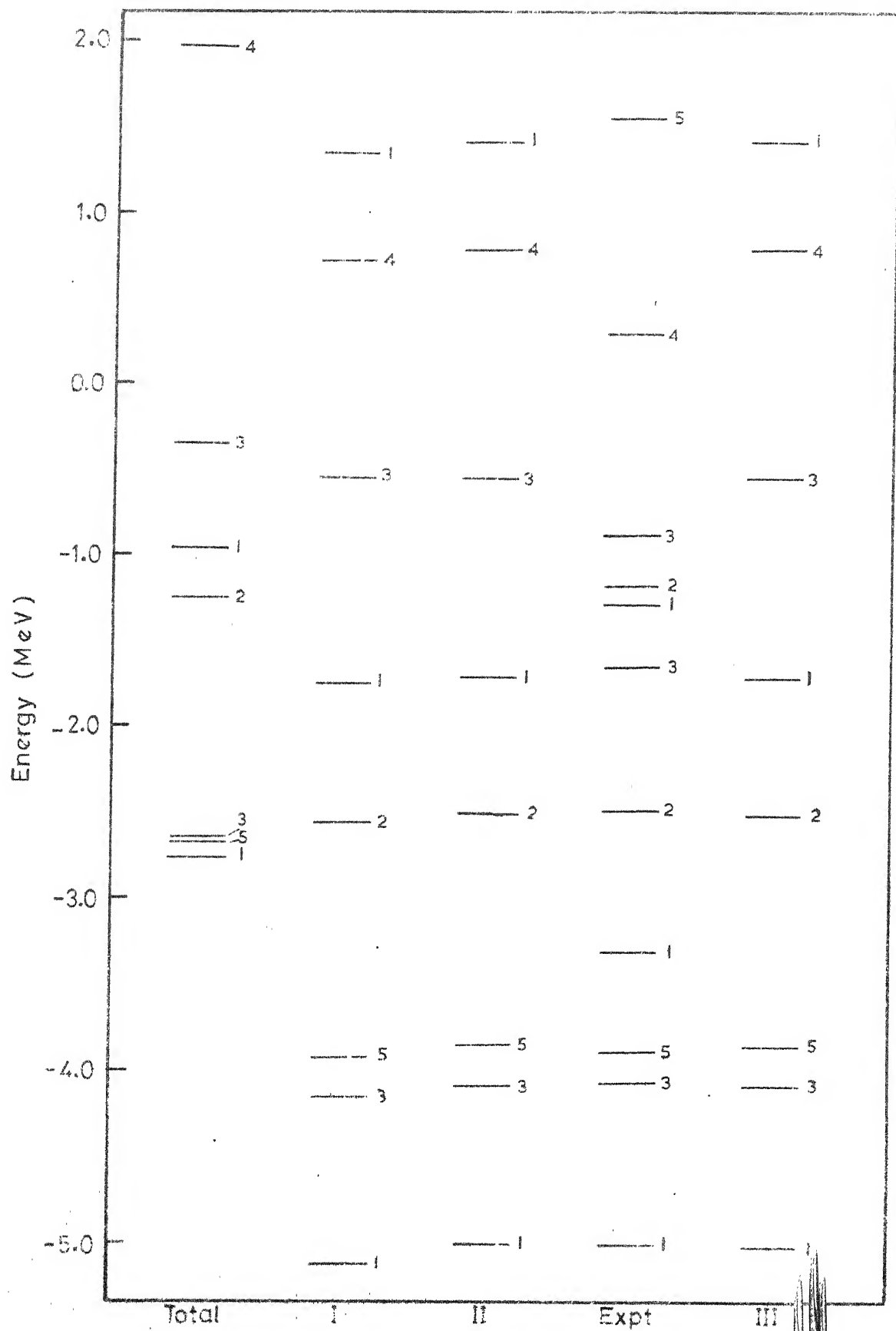


Fig. 2.18



TABLE 2.9

No.	$1^+$	$2^+$	$3^+$	$5^+$	$7^+$
EXP (MeV)	-2.563	0.606	-1.683	-1.663	-2.556
Bare (MeV)	-0.8484	1.0234	-0.6532	-0.9149	-1.7625
$\alpha$	0.5725	0.2435	0.6075	0.4775	0.4550
$\alpha_0$			0.50026		
Best fit (MeV) (with $\alpha_0$ )	-2.34924	0.11657	-1.50226	-1.70141	-2.63482
$\chi^2$ (MeV) <sup>2</sup>			0.29026		
$\alpha'_0$			0.54346		
Best fit (MeV) (with $\alpha'_0$ )	-2.48219	0.03207	-1.57343	-1.77054	-2.71016
$\chi^2$ (MeV) <sup>2</sup>			0.05386		

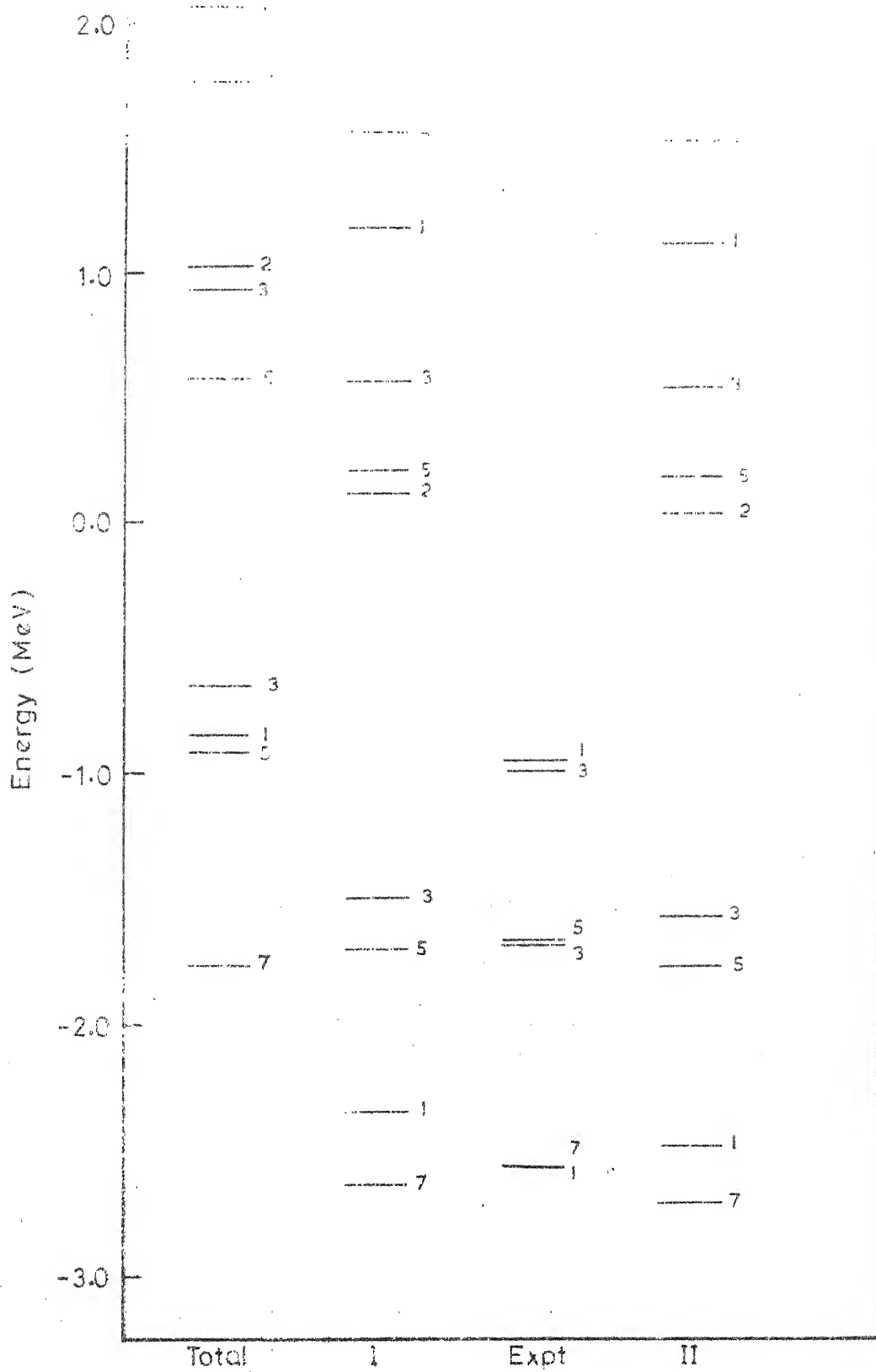


Fig. 2.19.

The observation when  $2^+$  level of  $^{18}\text{F}$  is excluded from the fit, the fit does not improve much - deserves further analysis. This level arises predominantly from the  $(1s_{1/2} \text{ } 0d_{5/2})$  configuration. The single particle energy of this configuration is about 0.7 MeV. Results improve in  $^{42}\text{Sc}$  also when the  $2^+$  level, which receives largest contribution from  $(1p_{3/2} \text{ } 0f_{7/2})$  configuration whose single particle energy is 2 MeV, is excluded from the fit. However, the improvement in  $^{42}\text{Sc}$  is not as much as it is in  $^{18}\text{F}$  on exclusion of  $4^+$  level which arises from  $(0d_{3/2} \text{ } 0d_{5/2})$  configuration whose single particle energy is about 5 MeV. The  $2^+$  level of  $^6\text{Li}$  can also be similarly discussed as it arises from  $(0p_{1/2} \text{ } 0p_{3/2})$  configuration with a single particle energy of 3.72 MeV. These all results mean that it is sufficient to change only the  $^3\text{S}_1$  matrix elements to get a renormalized force for levels arising from the lowest  $j^2$  configuration. This approach is also successful, to some extent, for levels arising from excited configurations with low single particle excitation energy. Further, mathematically it might be possible to find a reasonable value of  $\alpha$  for excited configurations with higher excitation energies. However, with such levels included, it is not possible to arrive at a best fit value of  $\alpha$  which would describe other low-lying levels as well as

can be done by excluding them. From Tables 2.8 and 2.9 we can see that this difficulty arises because the value of  $\alpha$  for such levels is much different from the ones for the lowest  $j^2$  configuration. For  $^{18}\text{F}$ , it can be seen that the value of  $\alpha$  for  $4^+$  level is much larger than those required for other levels. This might mean that the relative dominance of the  $^3\text{S}_1$  relative states in excited configurations is not as much as it is for the ground state configuration. However, then, we cannot explain how come is it that the  $2^+$  level of  $^{42}\text{Sc}$  can be explained by a much smaller value of  $\alpha$  than the others required for the ground state configuration levels.

We now discuss the results of calculation of pairing-plus-quadrupole renormalization of  $T = 1$  SME. The results are presented in Figures 2.20 - 2.23. In all these figures, modified energy levels, as a result of pure  $\delta$ -function force renormalization, are shown for even  $J$ 's only. The odd -  $J$  levels for whom the  $\delta$ -function force does not contribute are not shown. As explained, there were a large number of sets of strength variables possible each of which could give the correct ground state energy. However, in these figures, results are plotted only for those parameter sets, each of which could very well describe at least one excited level. The numerical results are given in Tables 2.10 - 2.13.

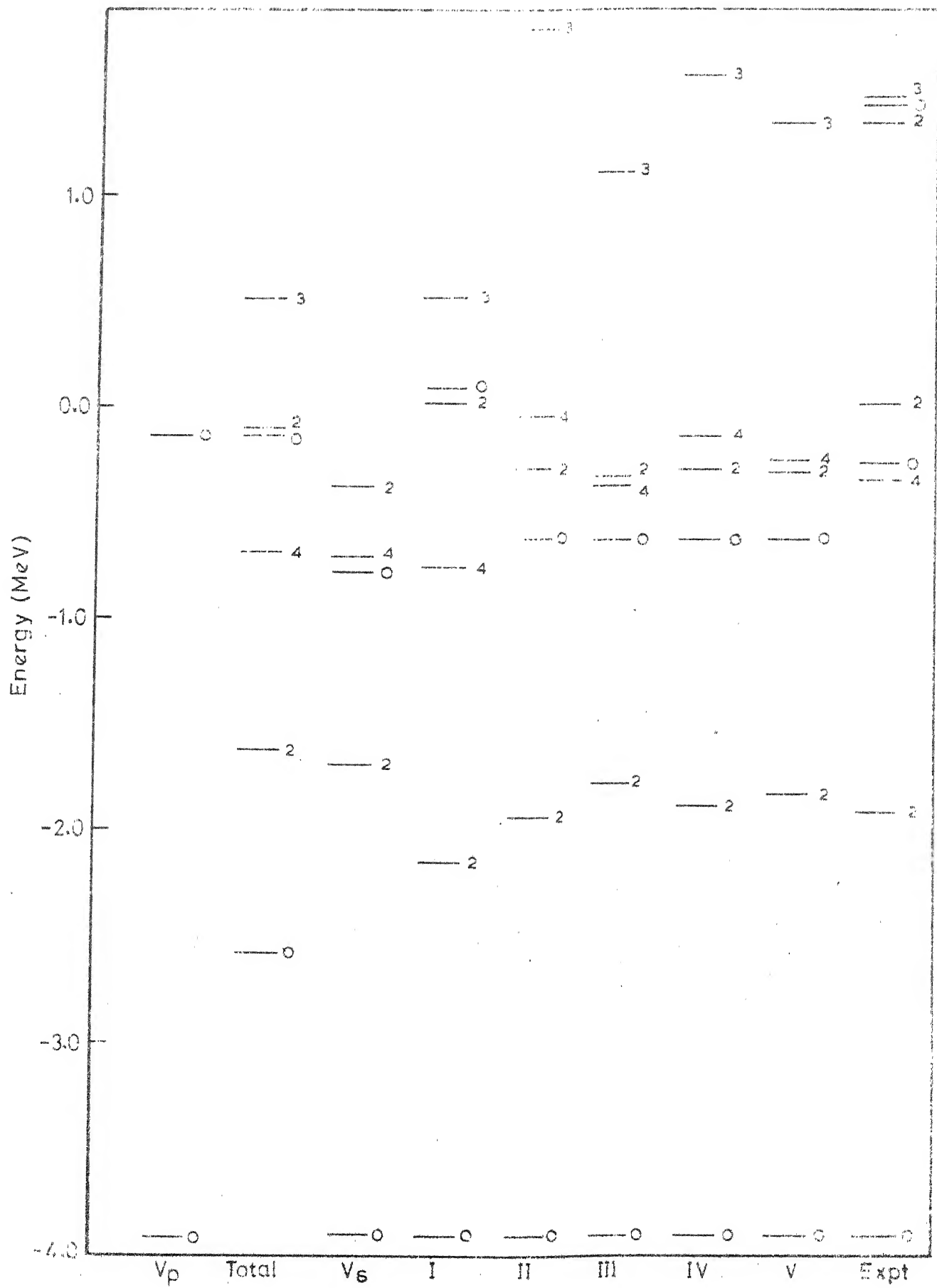


Fig. 2.20

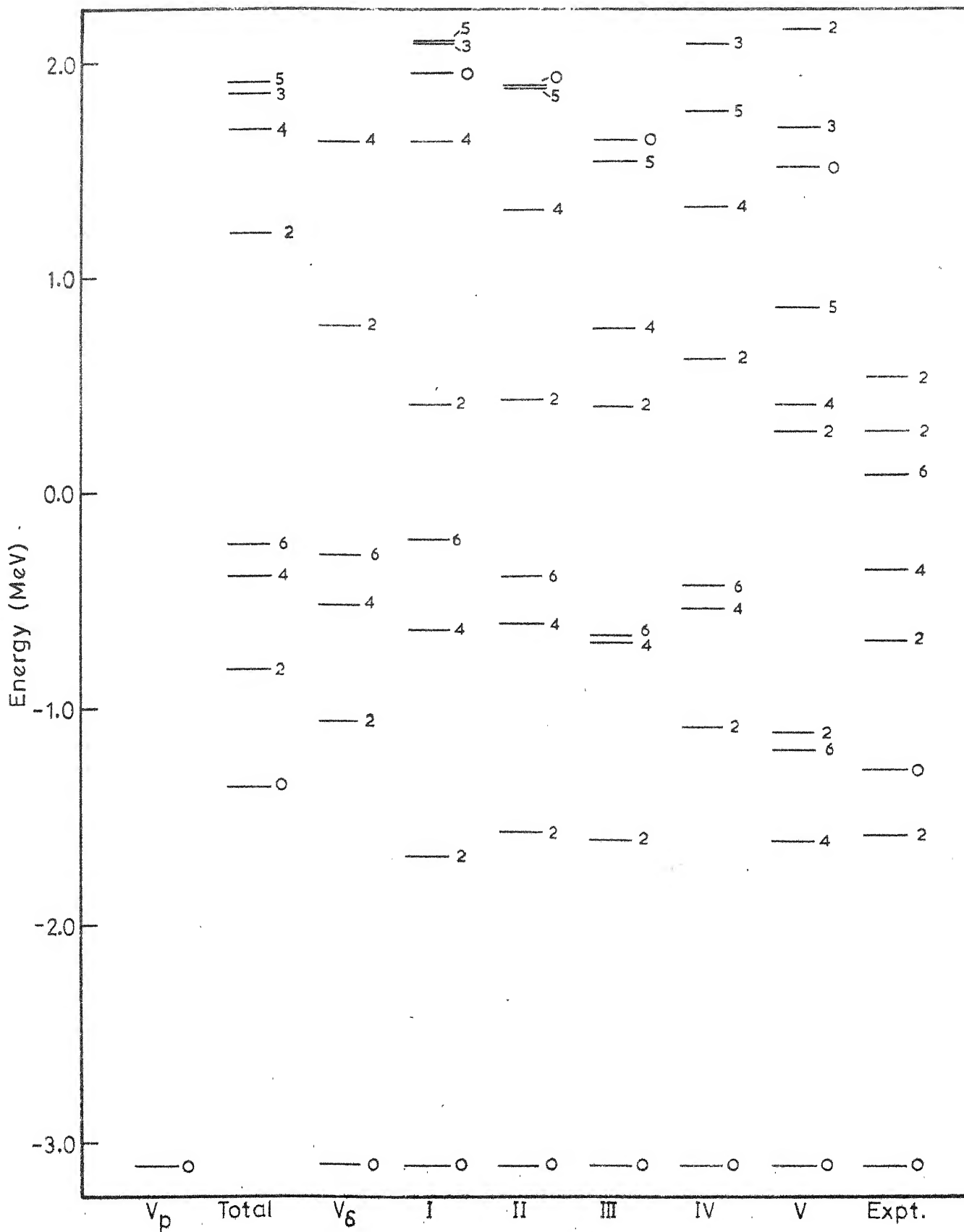


Fig. 2.21

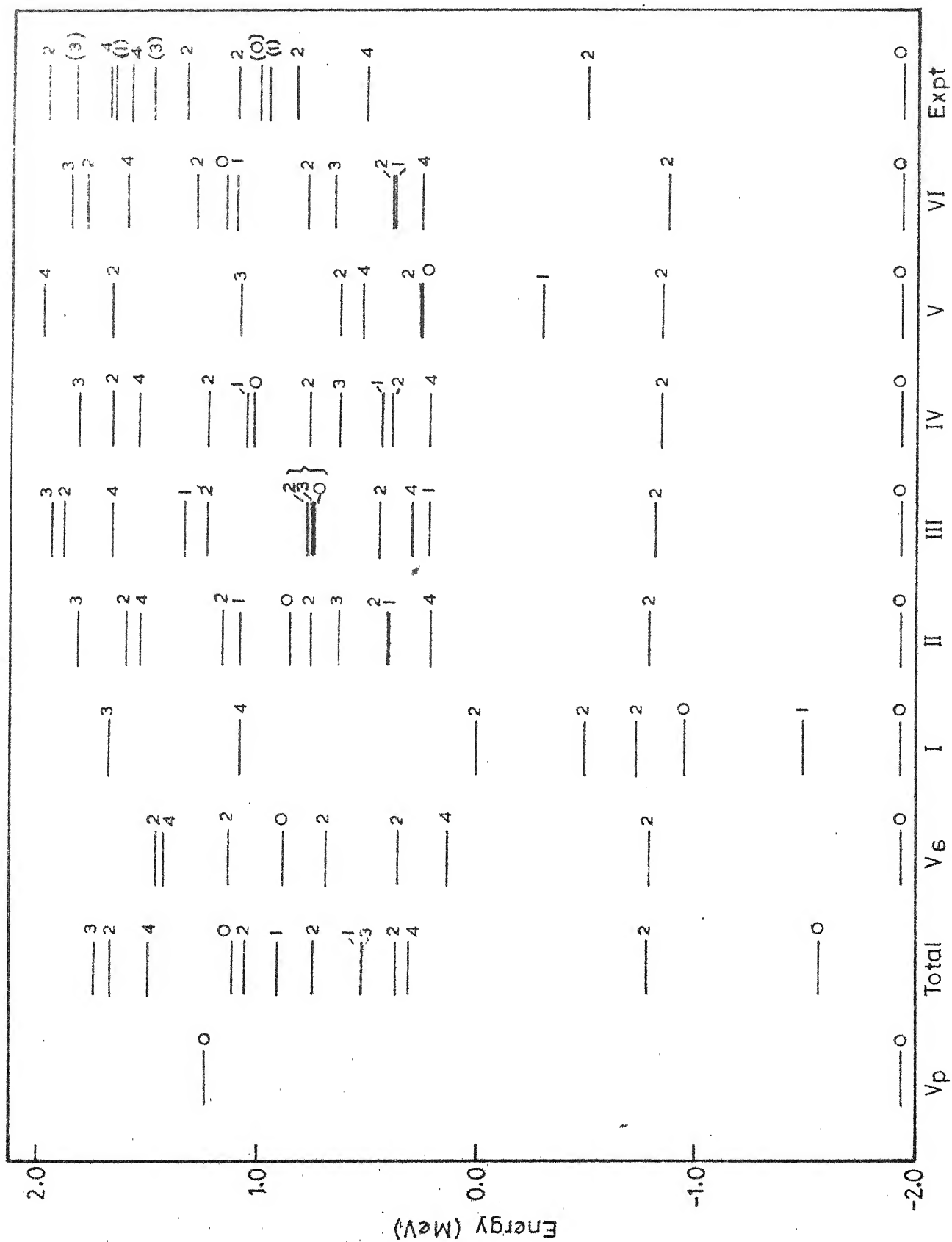


Fig. 2.22

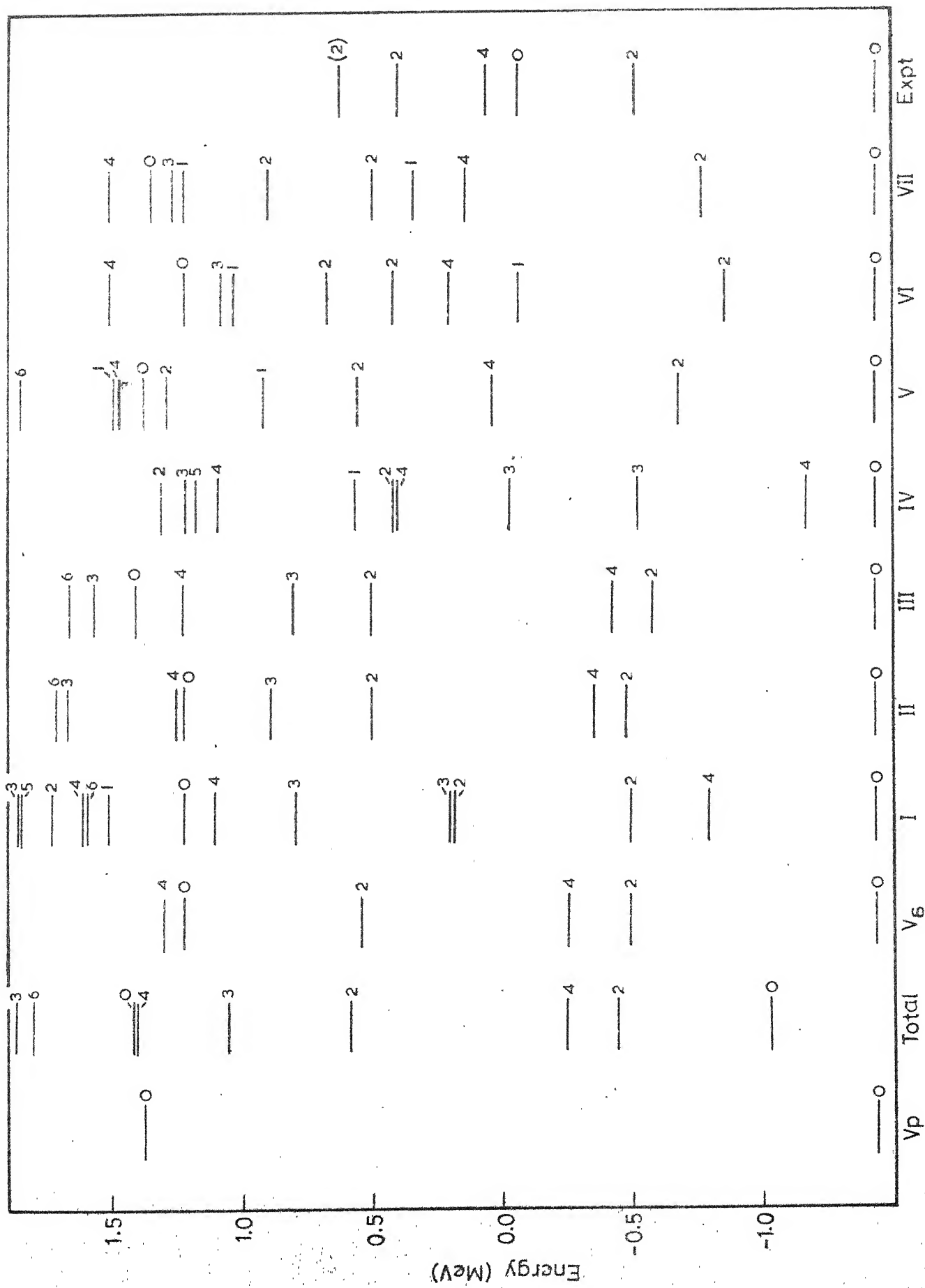




TABLE 2.10

Results of pairing - plus - quadrupole force renormalization of  $T = 1$  interaction in  $^{18}\text{O}$ . Columns I, II and III together, at any S.No. give, respectively, the  $\delta$ -function force strength ( $V_0$ ), the singlet quadrupole force strength ( $\chi_0$ ) and the triplet quadrupole force strength ( $\chi_1$ ). Each set predicts at least one level very well whose J is indicated in column IV. The corresponding predicted and experimental energies are given in Columns V and VI respectively. These results are besides the reproduction of ground state energy which is achieved with each set.

S.No.	III			IV J	V Predicted energy (MeV)	VI Experimental Energy (MeV)
	I $V_0$ (MeV-fm <sup>3</sup> )	II $\chi_0$ (MeV/fm <sup>4</sup> )	III $\chi_1$ (MeV/fm <sup>4</sup> )			
1	-32	-0.015	0	2	0.01979	0.0147
2	-85	0.0	-0.06089938	2	-1.94218	-1.9223
3	-91	0.0	-0.02808502	4	-0.37647	-0.3515
4	-87	0.0	-0.05030690	3	1.57245	1.4676
5	-89	0.0	-0.03953160	3	1.34622	1.4676

TABLE 2.11

Results of pairing - plus - quadrupole force renormalization of  $T=1$  interaction in  $^{42}\text{Ca}$ . For explanation of symbols refer to Table 2.10. For the  $4^+$  and  $6^+$  levels the prediction is not as satisfactory as for other levels but among all the parameter sets no better agreement than this could be achieved.

S.No.	I $V_0$ (MeV-fm <sup>3</sup> )	II $\chi_0$ (MeV/fm <sup>4</sup> )	III $\chi_1$ (MeV/fm <sup>4</sup> )	IV J	V Predicted Energy (MeV)	VI Experimental Energy (MeV)
1	-30	-0.0125	-0.00519877	6	-0.21695	0.081
2	-40	-0.0125	0.00107876	2	-1.56919	-1.589
3	-25	-0.0145	0.01047750	2	-1.60286	-1.589
4	-140	-0.0050	0.00405170	4	-0.53473	-0.359
5	-105	-0.0100	0.02969630	2	0.28066	0.281

TABLE 2.12

Results of pairing -plus - quadrupole force renormalization of  $T = 1$  interaction for  $^{58}\text{Ni}$ . For explanation of symbols refer to Table 2.10.

S.No.	I $V_0$ (MeV-fm <sup>3</sup> )	II $\chi_0$ (MeV/fm <sup>4</sup> )	III $\chi_1$ (MeV/fm <sup>4</sup> )	IV J	V Predicted Energy (MeV)	VI Experimental Energy (MeV)
1	-145	0.00072268	0.034823	2	-0.72447	-0.482
2	-145	-0.00072268	-0.00217697	2	0.76258	0.8393
				2	1.16876	1.1018
				2	1.59320	1.3275
3	- 95	-0.00144537	-0.00540794	2	0.78072	0.8393
4	- 80	-0.00144537	-0.0017731	0(?)	1.02383	1.0064
5	- 50	-0.00216805	-0.01475747	4	0.53039	0.5231
6	-10	-0.00216805	-0.00242387	2	0.78033	0.8393

TABLE 2.13

Results of pairing - plus - quadrupole force renormalization  
of  $T = 1$  interaction in  $^{92}\text{Zr}$ . For explanation of symbols refer to  
Table 2.10.

S.No.	I $V_0$ (MeV-fm <sup>3</sup> )	II $\chi_0$ (MeV/fm <sup>4</sup> )	III $\chi_1$ (MeV/fm <sup>4</sup> )	IV J	V Predicted Energy (MeV)	VI Experimental Energy (MeV)
1	-78	0	0.00606949	2	-0.48878	-0.49954
2	-75	0	0.00121312	2	0.50518	0.41330
3	-33	-0.0008	0.00184685	2	0.51433	0.41330
4	-33	0.0112	0.01071000	2	0.42234	0.41330
5	-24	-0.0008	-0.00544121	4	0.04245	0.06160
6	-12	-0.0008	-0.00992663	2	0.42422	0.41330
7	-18	-0.0008	-0.00806039	2	0.50775	0.41330

A study of Figure 2.20 reveals that the overall agreement of predicted spectrum with experimental one for  $^{18}\text{O}$  is achieved with parameter set  $(-80, 0, -0.0395316)$  at S.No. 5 of Table 2.10 i.e. spectrum V. Similarly, in  $^{42}\text{Ca}$ , spectrum II gives an overall best agreement. The case of  $^{58}\text{Ni}$  is the one of worst agreement that with all efforts even the  $2_1^+$  level could not be elevated beyond  $-0.72447$  MeV (spectrum I) while it greatly disturbed all other levels. In spectra II, III, IV and VI, an improved agreement of excited  $2^+$  experimental levels other than the  $2_1^+$  one is seen but we can not say if physics-wise also we are correct since we are not making a one-to-one correspondence between the calculated and experimental  $2^+$  levels. Instead, the said agreement is established if the  $2_2^+$  calculated level is ignored from the comparison and the  $2_2^+$  experimental level is compared with  $2_3^+$  calculated level. If the  $2_2^+$  experimental level is really a true two-particle configuration and if our comparison turns out to be correct on calculation of other properties of this level, this would mean that an experimental  $2^+$  level corresponding to  $2_2^+$  calculated level is yet to be observed. However, we would like to take the blame on ourselves. For this nucleus we have not been able to achieve even the correct renormalization for the  $2_1^+$  level (in other nuclei at least this has

been possible). We would rather like to say that our renormalization approach has failed for this nucleus. For few excited levels we have been able to get satisfactory numbers but we make a reservation to say if the predicted parameters also represent the truth. Although the  $4^+$  level is best reproduced in spectrum V, we can say that spectrum VI gives the more satisfactory agreement than any other set. The  $^{92}\text{Zr}$  nucleus also does not present a much happy situation. The  $2_1^+$  level is best predicted in spectrum I but only at the cost of all other levels. Instead, at least correct ordering is predicted in spectrum II by just a negligible sacrifice in the fit of  $2_1^+$  level. The spectrum IV describes the  $2_2^+$  level best but otherwise the situation is unrealistic - even the predicted  $2_1^+$  level goes below the ground state (not shown in figure). Overall, the spectrum V describes the levels best.

#### II.4 CONCLUSION:

Thus, mathematically at least, we have been able to represent the renormalizations required for few low-lying levels in terms of the matrix elements of the  $^3S_1$  relative state. A two-body matrix element is the final outcome of an interplay among several channels of interaction. This statement also holds for the renormalizing two-body matrix elements. Their representation by  $^3S_1$

relative matrix elements alone is an oversimplification of things. As such, it seems difficult at this stage if some detailed study of the renormalization could be made in the presently adopted simple minded approach.

In conclusion we say that our approach turned out to be much less successful for  $T=1$  levels than for  $T=0$  levels. For  $T=0$  levels we calculated  $\alpha$  for different levels separately and then found the best fit value of  $\alpha$ . Thus we used several levels for establishing the effective interaction. However, it can be seen that, at least for lowest  $j^2$  configuration levels, the values of  $\alpha$  as calculated for different levels are quite close and therefore, even if we had not used several levels, predicted excited levels, even calculated with  $\alpha$  as for ground state, would have been better described than with bare interaction. In case of  $T = 1$  levels, the attempt of determining three parameters by using only one experimental level turned out to be the root cause of troubles. We only tried to find parameters so that the ground state  $O^+$  level energy is correctly reproduced. However, in this process, it was never guaranteed that other levels would also be reproduced. Therefore, we had to scan the whole range of possible values of parameters in small steps with a hope that we might strike a parameter

set which is also suitable for description of higher levels. In first run, when the parameters were varied in crude steps, to see if such an approach is going to yield some results at all, such close agreement was not found because of which, in the final run, parameters were varied in finer steps. As per mathematical results, for  $T = 1$  levels, we have been able to predict the renormalization in terms of potential parameters for few of the low-lying states. Except for  $^{58}\text{Ni}$ , we have been able to reproduce at least the  $2_1^+$  level correctly, however, using only one level - the ground state  $0^+$ .



## CHAPTER III

### A PHENOMENOLOGICAL EFFECTIVE INTERACTION FOR $^{40}\text{K}$

#### III.1 INTRODUCTION:

Of the two nuclei  $^{40}_{19}\text{K}$  and  $^{38}_{17}\text{Cl}$ , the fact that energy levels of one could be derived if those of the other were known was one of the successes of  $jj$ -coupling nuclear shell model in its infancy. In their ground states, the  $^{40}\text{K}$  and  $^{38}\text{Cl}$  nuclei have respectively three and one protons in the  $\text{Od}_{3/2}$  orbit. Both of them have a single neutron in  $\text{Of}_{7/2}$  orbit. The low-lying energy levels of these nuclei are expected to arise as a result of interaction between the  $\text{Od}_{3/2}$  orbit protons and the lone neutron. Through the use of coefficients of fractional parentage, matrix elements of two-particle interaction in the configuration  $(\text{Od}_{3/2}^3 \text{Of}_{7/2})$  can be expressed as linear combinations of matrix elements of the same potential in the two-particle configuration  $(\text{Od}_{3/2} \text{Of}_{7/2})$ . This means that if same radial wave functions are assumed for the two nuclei (which amounts to assuming same oscillator length parameter  $b$  for them), energy levels of one can be derived if those of the other are known. The lowest four levels in both these

nuclei have  $J^\pi = 2^-, 3^-, 4^-$  and  $5^-$ . For  $^{38}\text{Cl}$ , these can be considered as coming from coupling the angular momentum  $3/2$  of the last proton to the angular momentum  $7/2$  of the odd neutron. If  $j-j$  coupling is valid for the valence nucleons, the three protons in the  $\text{Od}_{3/2}$  orbit, in compliance with the Pauli principle, can give a total angular momentum of  $3/2$  only and then the lowest four levels of  $^{40}\text{K}$  can also be considered as a result of coupling of the angular momentum  $3/2$  to  $7/2$ . Assuming these couplings, with a knowledge of excitation energies in  $^{40}\text{K}$  nucleus, it should be, then, possible to deduce excitation energies in  $^{38}\text{Cl}$  nucleus and their comparison with experimental spectrum of  $^{38}\text{Cl}$  will confirm the above assumptions. Goldstein and Talmi<sup>14</sup> found that the said transformation worked excellently.

The  $\text{Od}_{3/2}$  orbit can at most accommodate four particles and thus, the three protons in the  $\text{Od}_{3/2}$  orbit are equivalent to a vacancy - the hole - in the same orbit. Thus, the problem of handling three  $\text{Od}_{3/2}$  orbit protons and one  $\text{Of}_{7/2}$  neutron is mathematically equivalent to one of one hole and one particle. Pandya<sup>15</sup> showed that the matrix element of interaction between one hole-one particle states can be expressed as matrix elements of same interaction between two-particle states.

The relation he arrived at was

$$\begin{aligned}
 & \langle (j_h^{-1} j_p) JT | V | (j_h^{-1} j_p) JT \rangle \\
 &= - \sum_{J'T'} (2J'+1)(2T'+1) \begin{Bmatrix} j_h & j_p & J \\ j_h & j_p & J' \end{Bmatrix} \begin{Bmatrix} 1/2 & 1/2 & T \\ 1/2 & 1/2 & T' \end{Bmatrix} \\
 & \quad \langle j_h j_p J' T' | V | j_h j_p J' T' \rangle \quad (3.1)
 \end{aligned}$$

He also verified this relation for the case of  $^{40}\text{K}$  and  $^{38}\text{Cl}$  nuclei.

Since then, the problem of these two related nuclei has been discussed by different authors with different interactions. Kuo and Brown<sup>30</sup> calculated the spectra with reaction matrix derived from HJ potential. Dieperink et.al.<sup>59</sup> used Tabakin interaction and the modified surface delta interaction (MSDI) and worked both in TDA and RPA. Dieperink and Brussaard<sup>135</sup> have tried to parametrize the effective interaction in Talmi approach. Besides these specific nuclei, attempts have also been made of determining the  $d_{3/2} - f_{7/2}$  two-body interaction matrix elements from studies in neighbouring nuclei. Moinester and Alford<sup>136</sup> have determined the  $d_{3/2} - f_{7/2}$  interaction using multipole sum rule methods. Sartoris and Zamick<sup>57</sup> have shown that the discrepancy between

particle-hole matrix elements of nuclear interactions as obtained by using a realistic interaction and as derived from experiment is partly but not completely removed by considering the effects of core-polarisation. They had proved this statement by using HJ and KK interactions and with the  $Od_{3/2}$  and  $Of_{7/2}$  configurations as example. However, the paper was written in the year 1967 and today we know that microscopic core-polarisation calculations are not satisfactory. Erne<sup>137</sup> has discussed the problem of nuclei in the range  $^{33}\text{S} - ^{41}\text{Ca}$  under the assumption of an inert  $^{32}\text{S}$  core and, instead of using Pandya transformation, he has calculated the matrix elements for the  $Od_{3/2}^n Of_{7/2}$  configuration in terms of  $Od_{3/2} Of_{7/2}$  configuration particle-particle matrix elements which were then determined in Talmi approach.

In the past few years, several measurements of energy levels of  $^{40}\text{K}$  have been made and now we have a better knowledge of the energies and spin-parities of quite a few low-lying levels of this nucleus. In the previous chapter we have pointed out that the paucity of experimental information is the major obstacle in the way of determination of phenomenological effective interaction for any nucleus. As such, with the improved knowledge about the levels, prospects of establishing a reasonable

effective interaction today are brighter .

Johnson and Kennett<sup>138</sup> have determined level energies and deduced spin-parities of levels in  $^{40}\text{K}$ . Fink and Schiffer<sup>139</sup> have recently performed (d,p) experiments on  $^{37}\text{Cl}$  and  $^{39}\text{K}$  with 12 MeV deuterons.

In the previous Chapter we have seen that introduction of both phenomenological and experimental information into microscopic calculations improves the results and also makes them economic in respect of computer time. However, a comparison of the results for  $T = 0$  and  $T = 1$  states shows it clearly that the improvement depends upon the amount of information put in. Basically a realistic interaction is also derived through phenomenology. However, the amount of available experimental data is so vast that in construction of the phenomenological form of the free N-N interaction, we can incorporate as many dependences as we wish. Now, it is only speculation on our part that by addition of seemingly justifiable corrections we can modify it properly so as to be usable for calculation of bound state properties. Such an approach has ultimately been shown to have failed and, as discussed, the semi-microscopic approach has also not met enough success unless sufficient experimental information is fed into the calculation. Then it seems

to us that this semi-microscopic approach, a hybrid, is no better than the purely phenomenological approach to nuclear structure except for the fact that in the former, at least a part of the effective interaction is known to have some well-founded origin.

In the previous chapter we have used Sussex matrix elements (SME) under the assumption of their being composed of central, spin-orbit and tensor components. This interaction also gives gross similar results as other realistic interactions do and also, at least the study of spectra with the central, spin-orbit and tensor components did not lead us to any conclusion which might have made us feel doubtful as to the basic constitution of the interaction as regards its components. Thus, we feel that the true free N-N interaction, as represented by the SME, might be possessing several complicated dependences as evidenced by existence of such terms in other realistic interactions, yet, effectively it can be understood as consisting of central, spin-orbit and tensor components.

With above considerations in mind we believe that if parametrization of a phenomenological particle-particle interaction incorporating the central, spin-orbit and tensor dependences could be possible, it would be as

good as a semi-realistic interaction. At least it would be designed to reproduce experimental energies. For that matter, even realistic or semi-realistic interactions also do not guarantee wave functions. A purely microscopic approach does not lead us to the true numbers and once we start introducing phenomenology, there can be more than one ways, each of them being reasonable and sensible in its own place but different forms of addition will result in different structures of wave functions.

For the purpose of parametrizing a phenomenological effective interaction, we suppose, the  $^{40}\text{K} - ^{38}\text{Cl}$  nuclei present a favourable example. Now, sufficient experimental information about low lying levels of  $^{40}\text{K}$  is at hand so that an effective interaction, constructed from central, spin - orbit and tensor dependences of the N-N potential, can be tried to be parametrized. Enough experimental information is not available about  $^{38}\text{Cl}$  levels. Hence, the effective interaction parameters cannot be determined from known levels in  $^{38}\text{Cl}$ . However, as pointed out earlier, in eq. (3.1), the hole-particle interaction is same as the particle-particle interaction  $V$  for which the two-particle matrix elements, as appearing on the right of eq. (3.1), are calculated. Thus, once the parameterization is done for  $^{40}\text{K}$  levels, the energy levels of  $^{38}\text{Cl}$

are automatically calculated. We take this relation between the two sets of energy levels as the test of the effective interaction parameters. We find the best set of parameters for  $^{40}\text{K}$  and apply it to energy levels calculation in  $^{38}\text{Cl}$ .

### III.2 METHOD OF CALCULATION:

Bass and Wechsung<sup>140</sup> have tried to deduce the amount of configuration mixing from a study of electromagnetic transitions between negative parity states in  $^{40}\text{K}$  and they find that the structure of low lying levels can be reasonably described in terms of relatively simple configurations. Their results are shown in Table 3.1.

It, thus, becomes clear that, except for the excited  $3^-$  level, the wave functions are almost pure - a result perceived by Goldstein and Talmi much earlier. It presents a favourable situation for parametrizing a phenomenological effective interaction - at least the parameters obtained will not bear the blame of unduly absorbing large configuration mixing effects of configurations lying outside the model space. Although a model space allowing the hole to be anywhere in sd-shell and the particle to be anywhere in fp-shell would be much desirable yet, in view of available information about wave-functions.



TABLE 3.1

Relative intensities of component configurations in the structure of  $^{40}\text{K}$  levels as derived by Bass and Wechsung<sup>140</sup>.

Level energy (MeV)	$J^\pi$	Intensities (in per cent)			
		( $0d_{3/2}^{-1}$ $0f_{7/2}$ )	( $0d_{3/2}^{-1}$ $1p_{3/2}$ )	( $1s_{1/2}^{-1}$ $0f_{7/2}$ )	
0	$4^-$	100			
0.03	$3^-$	98	2		
0.8	$2^-$	99	1		
0.892	$5^-$	100			
2.048	$2^-$	3	97		
2.070	$3^-$	3	65	32	
2.104	$1^-$		100		
2.626	$0^-$		100		

we feel it would be reasonable enough to choose the smaller model space:

hole states :  $0d_{3/2}$ ,  $1s_{1/2}$

particle states:  $0f_{7/2}$ ,  $1p_{3/2}$

In principle, unless we show in our case also that the effect of left out configurations is really small, our assumption of this truncated space will remain questionable. However, upto the extent of nonaccountable effects of left out configurations on spectra calculated with effective interaction parameters derived in a truncated model space, we assume that the effective interaction will explain low-energy levels.

Goode and Zamick<sup>141</sup> have proposed two sets of single particle energies in this mass region

	SET I (MeV)	SET II (MeV)
$0d_{5/2}$	-11.7	-9.9
$1s_{1/2}$	- 9.7	-7.7
$0d_{3/2}$	- 7.2	-5.4
$0f_{7/2}$	0.0	0.0
$1p_{3/2}$	1.9	1.9
$1p_{1/2}$	4.25	4.25
$0f_{5/2}$	6.25	6.25
$\epsilon_{0f_{7/2}} - \epsilon_{0d_{3/2}}$	7.2	5.4
$\epsilon_{0d_{3/2}} - \epsilon_{1s_{1/2}}$	2.5	2.3

They observe that the spectra of  $^{39}\text{K}$  and  $^{41}\text{Ca}$  are insensitive to changes of 1 MeV or so in their single particle energies. Although the results in  $^{40}\text{Ca}$  are improved by decreasing the gap between  $0f_{7/2}$  and  $0d_{3/2}$  orbits from 7.2 to 5.4 MeV, the results in  $^{39}\text{K}$  and  $^{41}\text{Ca}$  deviate even more from the experimental values. Dieperink et.al.<sup>59</sup> have used a different set for  $^{40}\text{Ca}$  nucleus

TABLE 3.2

Experimental situation regarding energy levels  
in  $^{40}\text{K}$  as per different available compilations.

$J^\pi$	Ref. 138 Ex (MeV)	$J^\pi$	Ref. 142 Ex (MeV)	$J^\pi$	Ref. 139 Ex (MeV)
$4^-$	0	$4^-$	0	$4^-$	0
$3^-$	0.0296	$3^-$	0.0296	$3^-$	0.03
$2^-$	0.8	$2^-$	0.8001	$2^-$	0.801
$5^-$	0.892	$5^-$	0.8916	$5^-$	0.891
$2^-(3^-)$	2.0473	$2^-$	2.0474	$2^-$	2.048
$3^-$	2.0693	$3^-$	2.0697	$3^-$	2.072
$1^-(2^-, 3^-)$	2.1043	$(1)^-$	2.1036	$(1)^-$	2.105
$(2^-, 3^-)$	2.4188	$4^-$	2.3976	$4^-$	2.397
$3^-$	2.4575	$2^-$	2.4191	$2^-$	2.420
$1^-, 2^-, 3^-, 4^-)$	2.6265	$(0)^-$	2.6258	$(0)^-$	2.628
$1^-$	2.7301				
$1^-(2^-, 3^-)$	2.7562				
$2^-(3^-)$	2.7862				

Contd.

Ref. 138

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$2^-(3^-)$	2.8077
$2^-$	3.1283
$3^-$	3.3671
$1^-$	3.4387
$3^-$	3.4857
$3^-(2^-)$	3.6636
$1^-$	4.0198
$1^-$	4.1040
$1^-$	4.2536
$3^-$	4.4628
$1^-(2^-, 3^-)$	4.5378

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TABLE 3.3

Adopted level energies and prospective dominant configurations in the structures of respective levels.

Level number	$J^\pi$	Ex (MeV)		
1	$4_1^-$	0	$Od_{3/2}^{-1}$	$Of_{7/2}$
2	$3_1^-$	0.0296	$Od_{3/2}^{-1}$	$Of_{7/2}$
3	$2_1^-$	0.8	$Od_{3/2}^{-1}$	$Of_{7/2}$
4	$5_1^-$	0.892	$Od_{3/2}^{-1}$	$Of_{7/2}$
5	$2_2^-$	2.0473	$Od_{3/2}^{-1}$	$1p_{3/2}$
6	$3_2^-$	2.0693	$Od_{3/2}^{-1}$	$1p_{3/2}$
7	$1_1^-$	2.1043	$Od_{3/2}^{-1}$	$1p_{3/2}$
8	$3_3^-$	2.4575	$1s_{1/2}^{-1}$	$Of_{7/2}$
9	$2_3^-$	2.4191		
10	$4_2^-$	2.3976	$1s_{1/2}^{-1}$	$Of_{7/2}$
11	$0_1^-$	2.626	$Od_{3/2}^{-1}$	$1p_{3/2}$

function. The assignment to levels 1-4 is unique.

Excitation of the particle from  $Of_{7/2}$  to the  $1p_{3/2}$  orbit requires 1.9 MeV energy while 2.5 MeV are needed for exciting a hole from the  $Od_{3/2}$  to the  $1s_{1/2}$  orbit. We do anticipate a  $1^-$  level around 2 MeV energy as resulting from excitation of the particle to  $1p_{3/2}$  orbit while the hole stays in  $Od_{3/2}$  orbit. On the basis of this we assign configurations to levels 5-7. The  $Od_{3/2}^{-1} 1p_{3/2}$  configuration will give a  $0^-$  level also. On the basis of consideration of single particle (hole) energies, other  $0^-$  levels arising from  $1s_{1/2}^{-1} 1p_{1/2}$  and  $(Od_{5/2}^{-1} Of_{5/2})$  configurations are expected to lie much higher in energy. We assign this configuration  $(Od_{3/2}^{-1} 1p_{3/2})$  to level no.11. In the ascending order of unperturbed energies, next comes the configuration  $1s_{1/2}^{-1} Of_{7/2}$ . We assign this configuration to levels 8 and 10. However, this assignment is not expected to be very satisfactory since the unperturbed energy itself of the  $1s_{1/2}^{-1} Of_{7/2}$  configuration is 2.5 MeV while each of the  $3_3^-$  and  $4_2^-$  levels appears at an excitation energy less than 2.5 MeV which is possible only if the particle-hole interaction in this configuration is strongly attractive so that the unperturbed matrix elements of Hamiltonian for both these J states fall quite lower than 2.5 MeV since configuration mixing will send them up again. Or, may be

that there are other  $3^-$  and  $4^-$  unidentified levels which are causing configuration mixing. Otherwise, except for the possibility of some complicated configuration level getting down low in energy which might be a possible cause of this configuration mixing, there are no other  $3^-$  and  $4^-$  levels within the model space considered. Even otherwise, the unperturbed energies of  $\text{Od}_{3/2}^{-1} 1p_{3/2}$  and  $1s_{1/2}^{-1} \text{Of}_{7/2}$  configurations are 1.9 MeV and 2.5 MeV respectively - quite close. As such, we anticipate approximation of assigning pure configurations to  $3_2^-$  and  $3_3^-$  levels to be somewhat restricted. In comparison to the  $2_2^-$  level energy, the  $2_3^-$  level appears at much too low an excitation energy to be accounted for by some simple configuration like  $(\text{Od}_{3/2}^{-1} 1p_{1/2})$ ,  $(1s_{1/2}^{-1} 1p_{3/2})$  or  $(\text{Od}_{5/2}^{-1} \text{Of}_{7/2})$ . We do not include it in the fitting calculation. As more and more dependences in the effective potential are introduced, larger number of experimental levels are required. Attempt has been made to avoid use, as far as possible, of levels of uncertain configurations.

For  $^{40}\text{K}$ ,  $T = 1$ . Hence, using

$$\begin{Bmatrix} 1 & 1/2 & 1/2 \\ 0 & 1/2 & 1/2 \end{Bmatrix} = 1/2$$



and 
$$\begin{Bmatrix} 1 & 1/2 & 1/2 \\ 1 & 1/2 & 1/2 \end{Bmatrix} = 1/6$$

the matrix elements of Hamiltonian between one particle-one hole configurations are given by

$$\begin{aligned} \langle (j_h^{-1} j_p) J1 | H | (j_h^{-1} j_p) J1 \rangle &= \{ \epsilon_o + \epsilon_p - \epsilon_h \} \delta_{j_h j_h'} \delta_{j_p j_p'} \\ &- \frac{1}{2} \sum_{J'} (2J'+1) \begin{Bmatrix} j_h & j_p & J \\ j_h' & j_p' & J' \end{Bmatrix} \langle j_h, j_p J' 0 | V | j_h j_p, J' 0 \rangle \\ &- \frac{1}{2} \sum_{J'} (2J'+1) \begin{Bmatrix} j_h & j_p & J \\ j_h' & j_p' & J' \end{Bmatrix} \langle j_h, j_p J' 1 | V | j_h j_p, J' 1 \rangle \end{aligned} \quad (3.2)$$

where experimental values for single particle (hole) energies  $\epsilon_p$  ( $\epsilon_h$ ) are to be used. In the ground state configuration there is a hole in  $Od_{3/2}$  orbit and a particle in  $Of_{7/2}$  orbit and experimental excitation energies are known as relative to the  $4^-$  ground state level arising from this configuration. The gap between the  $Of_{7/2}$  and  $Od_{3/2}$  orbits is common to all levels and, hence, simply irrelevant for excitation energies relative to ground state. Like this, effectively the single particle energies needed in configurations  $(Od_{3/2}^{-1} 1p_{3/2})$  and  $(1s_{1/2}^{-1} Of_{7/2})$  are 1.9 MeV and 2.5 MeV respectively.

First we take the residual interaction as the pure central force

$$V_C(r) = \sum_{T,S}^{2T+1, 2S+1} P_{TS} \Lambda_{TS} e^{-(r^2/r_{0S}^2)} \quad (3.3)$$

where  $^{2T+1, 2S+1}P$  is the projection operator that projects out states of isospin  $T$  and spin  $S$ ,  $\Lambda_{TS}$  is the strength in the particular  $(T,S)$  channel of interaction and  $r_{0S}$  is range in the spin state  $S$  i.e. we assume an isospin-independent range. Matrix elements of  $V_C(r)$ , as a function of  $\lambda (= \frac{r_0}{\sqrt{2}b})$ , are calculated using the formula (A.30) given in appendix A. This is done in view of simple relation for Talmi integrals in terms of  $\lambda$

$$I_p = \left( \frac{\lambda^2}{1 + \lambda^2} \right)^{p + 3/2} \quad (3.4)$$

The r.m.s. charge radius of  $^{40}\text{Ca}$  is 3.5 fm so that the corresponding value of  $b$  comes out to be 2.018635 fm. We take  $b = 2.0$  fm for  $^{40}\text{K}$ . Thus, after  $\lambda$  is determined, the range can be calculated from

$$r_{0S} = 2\sqrt{2} \lambda_S \quad (3.5)$$

Thus, there are six parameters specifying the central force. However, we have been able to reduce

the effective number of unknown parameters to four. This has been possible since we have an idea of the upper and lower limits for the nuclear force range  $r_0$ . We let  $\lambda_S$  (for both  $S = 0$  and  $S = 1$ ) vary independently between 0.3 and 1.5 in steps of 0.1 in first run. Thus, for a given  $(\lambda_0, \lambda_1)$  set the number of unknown parameters is reduced to four. In principle, four unknowns can be determined from a knowledge of four experimental values. However, in the present case we can find four  $A_{TS}$  parameters for each  $(\lambda_0, \lambda_1)$  set. Each set of the  $A_{TS}$  parameters obtained in this way will describe the four experimental values considered equally well and it will not be possible to distinguish the true set which will also be good for prediction of higher levels. To avoid it, for every  $(\lambda_0, \lambda_1)$  set, we minimise the function

$$\chi^2 = \sum_i \frac{(E_{i,Calc.} - E_{i,exp.})^2}{E_{i,exp.}} \quad (3.6)$$

for five excitation energies. The  $E_{i,cal}$ 's are the calculated excitation energies corresponding to the respective experimental excitation energies  $E_{i,exp}$ 's. For a given  $(\lambda_0, \lambda_1)$  set,  $E_{i,calc}$ 's are linear functions of all the four  $A_{TS}$ 's. The unknown strengths are determined by imposing mathematical restriction of  $\chi^2$

being minimum with respect to each  $A_{TS}$ .

An experimental energy level carries in itself the effect of so many off-diagonal matrix elements of the Hamiltonian matrix. If the Hamiltonian matrix is of dimensionality greater than two, it is not possible to write down an explicit analytic expression for perturbed energy eigenvalues in terms of off-diagonal and unperturbed diagonal matrix elements. We, therefore, have to resort to approximate methods. We assume that in first approximation the excitation energy of a level can be approximated by the difference of diagonal matrix element of Hamiltonian in that particular state and the diagonal matrix element of Hamiltonian for the ground state  $4^-$  level, in the limit of pure configurations. Fortunately, for this particular nucleus, it happens to be a very good approximation except for the 2.0693 MeV  $3_2^-$  level, (Cf. results of Bass and Wechsung<sup>140</sup>). In this manner it was found that the value of  $\lambda_0$  around 0.3 - 0.4 and that of  $\lambda_1$  around 1.1 - 1.2 gave the best agreement for the five excitation energies under consideration. After this,  $\lambda_0$  was varied between 0.3 and 0.4 and  $\lambda_1$  between 1.1 and 1.2, both in steps of 0.01, and the above procedure repeated for determining the strength parameters. Thus, the best set of strengths was chosen which gave least value of  $\chi^2$ .

However, it was found that, for a variation of 0.01 or so in  $\lambda_S$ ,  $\chi_{\min}^2$  was not sensitive enough although the strengths predicted, for such two successive sets of values of  $\lambda_S$ , were different. Thus, it became obvious that small changes in the range can be adjusted through a variation in strengths. For the same reason, no finer variations in  $\lambda_S$  were tried.

However, as we have said, true energy levels require an exact diagonalization to be made and also otherwise there is no way to distinguish which one of the two or more sets, which all give the same minimum  $\chi^2$ , is better. Furthermore, a set of parameters may give a least value of  $\chi^2$  in case of pure configurations. However,  $\chi^2$  obtained on diagonalization with this parameter set, may not be the minimum obtainable  $\chi^2$ . Still, in view of the earlier observation that this nucleus is a case of pure enough configurations we felt that a parameter set that gives minimum  $\chi^2$  on diagonalization would not be very much different from the one that gives minimum  $\chi^2$  for pure configurations. Therefore, besides the sets which gave minimum  $\chi^2$  for pure configurations, we also picked up other few which gave a  $\chi^2$  value not very much different from  $\chi_{\min}^2$ . The Hamiltonian matrices are then set up for all J states

in the model space  $(1s_{1/2}^{-1} \text{ } 0d_{3/2}^{-1} \text{ } 0f_{7/2} \text{ } 1p_{3/2})$  for each parameter set separately and diagonalized. The value of  $\chi^2$  is calculated again for the same five excitation energies, this time with calculated perturbed energy eigenvalues, with each parameter set. The different parameter sets, although may give same  $\chi^2$  for pure configurations, will contribute differently to off-diagonal matrix elements. This difference will show up in the value of  $\chi^2$  obtained for perturbed eigenvalues. The set which gives a minimum value of  $\chi^2$  is thus taken as the best representative of effective interaction parameters for the five excitation energies. However, derivation of a set of parameters, which give the best description of the variables used in determining them, is not all that is expected of an effective interaction. Instead, besides the known quantities used in determining the parameters, the interaction should also satisfactorily reproduce other quantities. In the present case this means that besides the five excitation energies employed in parameterizing the effective interaction, the parameter set should also satisfactorily predict the excitation energies of higher levels. It then turns out that the parameter set which gives a least  $\chi^2$  does not also describe other excited levels equally well as can be done by sacrificing

the value of  $\chi^2$  by a small amount. We, finally, select only that set which gives an overall best agreement with levels' excitation energies.

After the work with the central force is over, we proceed to determine the effective interaction parameters for a two-body potential of the form - a central force + a two-body spin-orbit force. The spin-orbit force

$$V_{LS}(r) = \sum_T \frac{2T+1,3}{P} S_T \vec{\ell} \cdot \vec{S} e^{-r^2/r_{LS}^2} \quad (3.7)$$

contributes to spin - triplet states only. Therefore, the central force parameters already determined will be no good for the central part of this combination since addition of the spin-orbit part will modify the spin-triplet central effective interaction. Then, to restore the fit, the central part will also have to be modified. We assume isospin (T) dependence of the spin-orbit force strength  $S_T$ . The matrix elements of this force are calculated using formula (A.36) given in appendix A.

Besides strengths, we have no reason to believe that the  $S = 0$  and  $S = 1$  central force range parameters  $\lambda_0$  and  $\lambda_1$  will also not change as a result of addition of the spin-orbit part. Instead, the modification

in central effective interaction might as well be reflected both in range, as well as in strength parameters. However, it is rather firmly established that the central part constitutes the major and most important part of the two-body effective interaction with spin-orbit and tensor parts providing finer details of the spectra. This we have also seen in Chapter II in connection with our study of relative importance of central, spin-orbit and tensor parts of Sussex matrix elements. As such, we assume that  $\lambda_0$  and  $\lambda_1$  will lie between 0.3 and 0.4 and between 1.1 and 1.2 respectively and, as earlier, we let them vary in steps of 0.01. The inclusion of spin-orbit part increases the number of unknown parameters from four to six and therefore two more experimental energy levels are needed. The spin-orbit force is operative in spin-triplet states only and hence, the range of this part is also expected to be round about the range of central part in triplet state. Therefore, for the spin-orbit part, we let  $\lambda'$ , defined through

$$r_{LS} = 2 \sqrt{2} \lambda' \quad (3.8)$$

vary from 1.1 to 1.355 in steps of 0.015. For each set of  $\lambda_0$ ,  $\lambda_1$  and  $\lambda'$ , the six strength parameters are calculated through the least square fitting procedure as described above.



The same procedure was repeated for parametrizing the effective potential of the form central + tensor. The form of the tensor force is

$$V_{\text{Ten.}} = \sum_T^{2T+1, 3} P S_T' \left[ \frac{3(\vec{\sigma}_1 \cdot \vec{r})(\vec{\sigma}_2 \cdot \vec{r})}{r^2} - (\vec{\sigma}_1 \cdot \vec{\sigma}_2) \right] e^{-(r^2/r_{\text{Ten.}}^2)} \quad (3.9)$$

where isospin (T) dependence of the strength  $S_T'$  is assumed. Two-body matrix elements of the tensor force are calculated using the formula (A.40) given in appendix A. The range parameter  $\lambda''$  as defined by

$$r_{\text{Ten.}} = 2\sqrt{2} \lambda'' \quad (3.10)$$

was varied from 1.1 to 1.205 in steps of 0.015. Still higher values of  $\lambda''$  were not tried so as to save computer time and the trend of  $\chi^2$  for pure configurations was identical with that for inclusion of the spin-orbit part and it was realized that with such low sensitivity of  $\chi^2$  to  $\lambda''$ , extension of it to still higher range of values will not bring any significant change in the final results on diagonalization.

We need five excitation energies for parametrization of pure central force. We take the  $4_1^-$

(ground state),  $3_1^-$  (0.0296 MeV),  $2_1^-$  (0.8 MeV),  $5^-$  (0.892 MeV),  $1_1^-$  (2.1043 MeV) and  $0_1^-$  (2.626 MeV) levels. For the inclusion of spin-orbit and tensor parts we consider the  $2_2^-$  (2.0473 MeV) and  $3_2^-$  (2.0693 MeV) levels also.

Now we proceed to parametrize the effective potential in the form central + spin-orbit + tensor. Thus, there are eight strength parameters requiring a knowledge of nine excitation energies, that is, ten level energies including the ground state. However, only eight excitation energies were available (the  $4_2^-$  level at 2.3976 MeV was established later). The  $3_3^-$  level at 2.4575 MeV was the only other, hitherto unused, level which could be used with some reasonable degree of definiteness as regards the main component in the wave function. Therefore, we had to resort to one more approximation. We assumed spin-isospin-dependence of strength and spin-dependence of range of central part (four parameters). We also assumed isospin-dependence of strength of spin-orbit part (two parameters more). In analogy with the spin-orbit part, it would be desirable to include isospin-dependence of strength of the tensor force part. However, we assumed that, on the basis of our previous knowledge that exact fixation

of strength and range is rather arbitrary and it is rather a joint contribution of the two which is parametrized, the isospin-dependence of the strength of the tensor force can be absorbed by taking ranges in the two isospin states to be different and assuming that the strength in both the isospin states is same. Like this the number of strength parameters was effectively reduced to seven although letting the range parameters for the two isospin states vary independently increased the computer time. However, the seven parameters could now be determined in a least square fitting procedure from a knowledge of eight excitation energies. We used the  $3\bar{3}$  level for fitting, besides the eight others mentioned above.

Thus, instead of the tensor potential as expressed in the form in eq. (3.9) we use in the form

$$V_{\text{Ten.}} = \sum_T 2T+1, 3 P S'' \left[ \frac{3(\vec{\sigma}_1 \cdot \vec{r})(\vec{\sigma}_2 \cdot \vec{r})}{r^2} - (\vec{\sigma}_1 \cdot \vec{\sigma}_2) \right] e^{-(r^2/r_{\text{Ten.,T}}^2)} \quad (3.11)$$

and correspondingly

$$r_{\text{Ten.,T}} = 2\sqrt{2} \lambda_T''' \quad (3.12)$$

The central force range parameters  $\lambda_S$  were varied between 0.3 and 0.4 and between 1.1 and 1.12 in

steps of 0.01 for  $S = 0$  and  $S = 1$  respectively. The range parameter  $\lambda'$  for the spin-orbit part was restricted to three values 1.1, 1.115 and 1.13. In the first run, for  $\lambda_0 = 0.3$ ,  $\lambda_1'''$  was assigned value 1.1, 1.115, 1.13 and 1.145 in succession and it was found that  $\chi^2$  was very sensitive towards the change of  $\lambda_1'''$  from 1.13 to 1.145, becoming much worse for  $\lambda_1''' = 1.145$ . Similar behaviour was observed in case of  $\lambda_0'''$  although the  $\chi^2$  was not so sensitive. Therefore, from  $\lambda_0 = 0.31$  onwards,  $\lambda_T'''$  (both for  $T = 0$  and  $T = 1$ ) were varied independently over three values 1.1, 1.115 and 1.13. Fixation of  $\lambda_1$  in the much smaller range (1.1 - 1.12) was intuitively done in view of the earlier observation that with central + spin-orbit and central + tensor forms,  $\lambda_1$  was predicted to be 1.1.

Twelve energy levels for  $^{40}\text{K}$  are expected to arise within the chosen model space. Out of these, we have used nine for determination of parameters. As discussed, a serious attempt of comparison of calculated  $4_2^-$  with experimental  $4_2^-$  level should not be made. In the energy region, around 4.5 MeV, where we expect the  $1_2^-$  and  $2_3^-$  levels arising from the  $(1s_{1/2}^{-1} 1p_{3/2})$  configuration to lie, the spin assignments are uncertain and there are several levels suspected to be  $1^-$  and  $2^-$ .

Hence, a reasonable comparison of predicted energies of these states is not possible.

However, in the process of establishing effective interaction for  $^{40}\text{K}$ , the two-particle matrix elements in the same model space as the one considered for particle-hole states are automatically calculated and the parameters can, thus, be verified against energy levels of  $^{38}\text{Cl}$ , predicted in the model space

proton :  $\text{Od}_{3/2}$

neutron:  $\text{Of}_{7/2}, \text{1p}_{3/2}$

The experimental energy levels of  $^{38}\text{Cl}$  are

$J^\pi$	Energy (MeV)
$2^-$	0
$5^-$	0.67127
$3^-$	0.75526
$4^-$	1.30887
$3^-$	1.61721
$3^-$	2.74310

The lowest four levels are precisely the ones that would be expected from the  $\text{Od}_{3/2} \text{Of}_{7/2}$  configuration.

However, appearance of two low-excited  $3^-$  levels makes it much doubtful if the simple two-particle model will work for them as it is expected to be for the lowest four  $Od_{3/2} Of_{7/2}$  configuration levels. The  $3^-$  level <sub>2</sub> appears at an excitation energy of 0.86195 MeV above the  $3^-$  level whereas an excited  $3^-$  state is expected from the  $Od_{3/2} 1p_{3/2}$  configuration for which the single particle excitation energy above the lowest  $Od_{3/2} Of_{7/2}$  configuration is not known since the levels of  $^{37}S$  and  $^{37}Cl$  are not established. However, taking same single particle energies as those taken for  $^{40}K$ , the single particle excitation energy of this configuration is 1.9 MeV. On the basis of this we expect the excited  $3^-$  states to have complicated structure rather than just two-particle states. We shall only see how well are the lowest four levels of  $^{38}Cl$  predicted with an effective interaction parameterized for  $^{40}K$ .

The  $^{38}Cl$  nucleus is one with neutron excess and hence the wave functions do not have pure isospin. Instead, we write a total angular momentum ( $J$ ) coupled proton-neutron state as  $|a(p)b(n)J\rangle$  where the proton is in single particle configuration  $a$  and the neutron is in the single particle configuration  $b$ . This state is obtained from states of well defined isospins through

$$|a(p) b(n) J \rangle = \frac{1}{\sqrt{2}} \left[ |a b J T \rangle_{T=1} + |abJT \rangle_{T=0} \right]$$

Therefore, a proton - neutron interaction matrix element will be

$$\begin{aligned} \langle a(p)b(n)J | V | c(p)d(n)J \rangle = & \frac{1}{2} \left[ \langle abJT | V | cdJT \rangle_{T=1} \right. \\ & \left. + \langle abJT | V | cdJT \rangle_{T=0} \right] \end{aligned}$$

Therefore, particle-particle matrix elements of  $T = 0$  and  $T = 1$  states (which have already been calculated during calculations for  $^{40}\text{K}$ ) for the appropriate configurations in the model space as considered for  $^{38}\text{Cl}$  are picked up and the Hamiltonian matrices for different  $J$  states constructed by taking averages of corresponding matrix elements in  $T=0$  and  $T=1$  states which are then diagonalized to get the energy levels of  $^{38}\text{Cl}$ .

### III.3 RESULTS AND DISCUSSION:

As discussed, six experimental levels were used for parameterization of the pure central force and there remained three more levels which were to be predicted with the parameters which gave best fit (i.e. minimum  $\chi^2$ ) for the six levels used. Therefore, it was for central

part only that the said six levels were best reproduced for the  $(\lambda_0, \lambda_1)$  set at values (0.39, 1.11) while the overall agreement with experimental spectrum including the other excited states also was obtained for the values (0.38, 1.14). Otherwise, for parametrization in the form central + spin-orbit and central + tensor, eight levels were already used for parametrization and there was not much point in seeking the fit for the  $3_3^-$  level for reasons discussed above. As such, for parametrization of the effective potential in these two forms, the particular set that gave an overall fit with the spectrum was identical with the one which gave a minimum  $\chi^2$  for the eight levels used. For the parametrization in the form central + spin-orbit + tensor, all the known nine levels were used up in parametrizing the potential and hence, for this form also, there was one unique set of parameters which gave minimum value of  $\chi^2$ .

The effective interaction parameters are shown in Table 3.4. The calculated, pure and configuration mixed levels for central potential as calculated with both the parameter sets are given in Table 3.5. Similar results for effective potentials in the other forms are presented in Table 3.6. The value of  $\chi_{\min}^2$  obtained in each case is also indicated. The same results are plotted in Figures 3.1 and 3.2. The wave functions as obtained



TABLE 3.4

S.No.	Interaction	Central		Central + spin - orbit	Central + tensor	Central + Spin-orbit + tensor
	Parameters	I	II			
1	$\lambda_0$	0.39	0.38	0.39	0.3	0.39
2	$\lambda_1$	1.11	1.14	1.10	1.10	1.10
3	$A_{00}(\text{MeV})$	-154.9	-218.7	-694.9	1337.50	590.80
4	$A_{01}(\text{MeV})$	-19.3	-20.0	-30.2	19.4	6.10
5	$A_{10}(\text{MeV})$	-90.1	-89.7	-39.0	-944.5	-342.50
6	$A_{11}(\text{MeV})$	-15.1	-13.5	-4.2	-50.8	-35.90
7	$\lambda'$			1.235		1.13
8	$S_0(\text{MeV})$			-1.1		-1.90
9	$S_1(\text{MeV})$			-8.3		11.40
10	$\lambda''$				1.115	
11	$S'_0(\text{MeV})$				-1.500	
12	$S'_1(\text{MeV})$				5.500	
13	$\lambda'''_0$					1.10
14	$\lambda'''_1$					1.13
15	$S'''_0(\text{MeV})$					-0.3
16	$S'''_1(\text{MeV})$					0.3
17	$r_{00}(\text{fm})$	1.103	1.0748	1.103	0.84851	1.103
18	$r_{01}(\text{fm})$	3.1395	3.2243	3.1113	3.11130	3.1113
19	$r_{LS}$ "			3.4932		3.1962
20	$r_{\text{Ten.}}$ "				3.1537	
21	$r_{\text{Ten.},0}(\text{fm})$					3.1113
22	$r_{\text{Ten.},1}$ "					3.1962

TABLE 2.2

S.No.	Expt. (MeV)	$J^{\pi}$	SET A		SET B	
			I (MeV)	II (MeV)	I (MeV)	II (MeV)
1	0	$4^{-}$	0	0	0	0
2	0.0296	$3^{-}$	0.02851	-0.0439	0.02846	-0.04488
3	0.8	$2^{-}$	0.80083	0.73161	0.80069	0.72810
4	0.892	$5^{-}$	0.88858	0.91340	0.88851	0.91203
5	2.1043	$1^{-}$	2.19636	2.17624	2.19641	2.17156
6	2.626	$0^{-}$	2.59049	2.61531	2.59147	2.61499
7	2.0473	$2^{-}$	1.95345	2.00975	1.96377	2.01898
8	2.0693	$3^{-}$	2.80860	2.67310	2.82108	2.68478
9	2.4575	$3^{-}$	3.46823	3.75060	3.50228	3.78248
10	2.3976	$4^{-}$	4.26282	4.31246	4.32430	4.37134
11		$1^{-}$	5.88799	5.95775	5.95850	6.03039
12		$2^{-}$	4.87027	4.95765	4.90651	4.99446
$\chi^2$			0.00456	0.19137	0.00454	0.19677

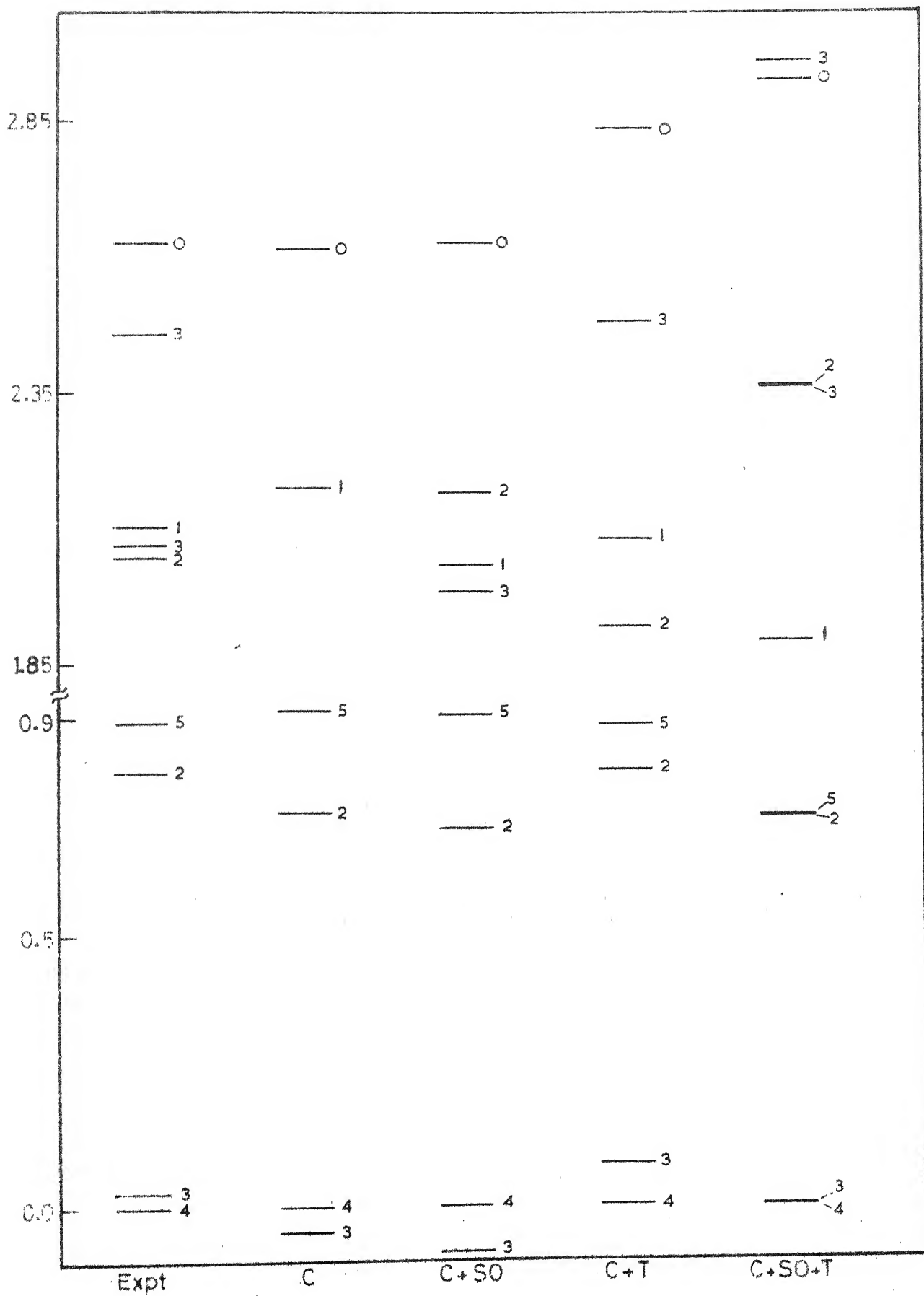


Fig. 3.1.

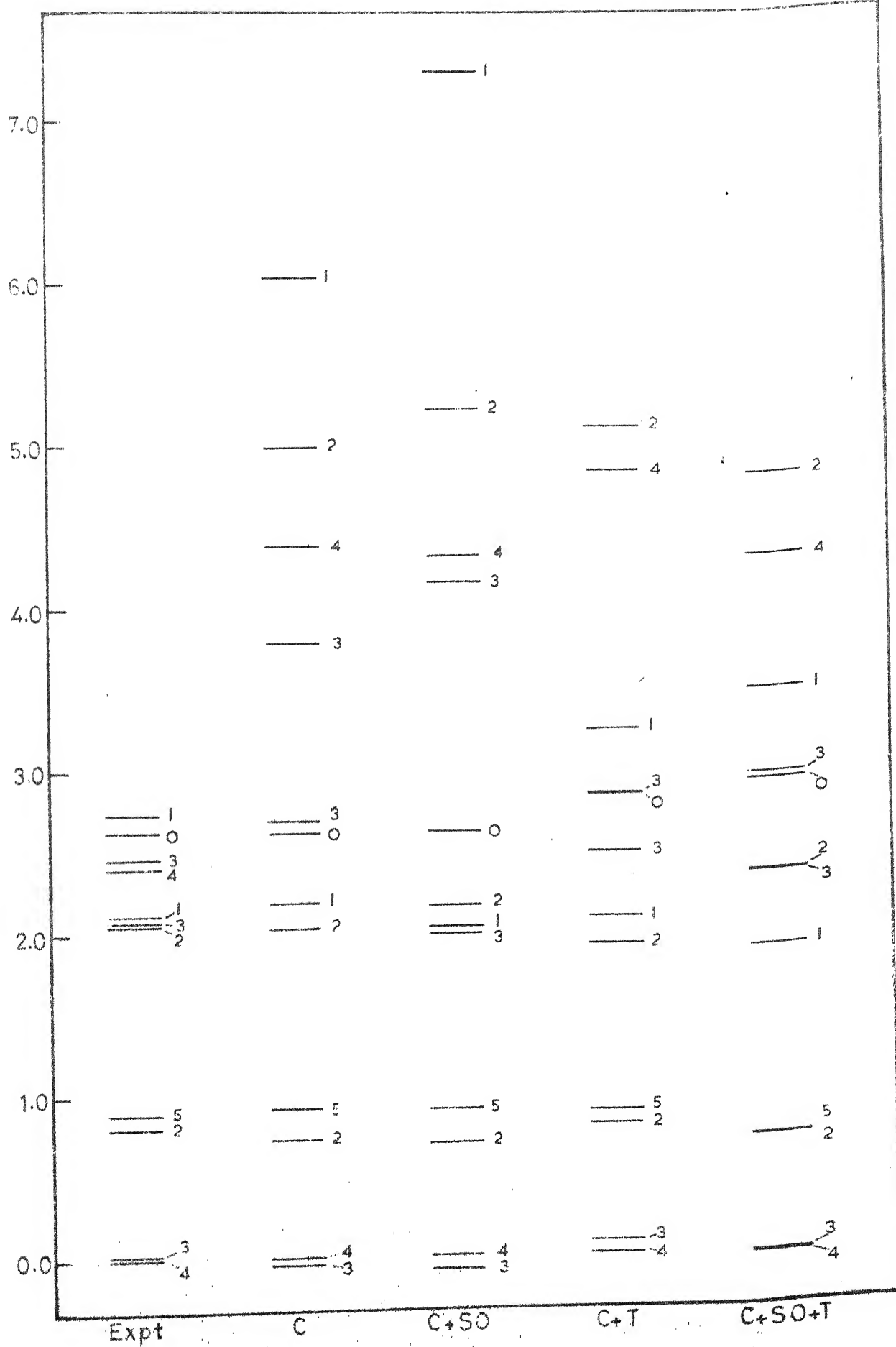


Fig.3.2.

TABLE 3.6

S.No.	Expt. (MeV)	$J^\pi$	Central+spin-orbit		Central + tensor		Central+spin-orbit+tensor	
			I (MeV)	II (MeV)	I (MeV)	II (MeV)	I (MeV)	II (MeV)
1	0	$4^-$	0	0	0	0	0	0
2	0.0296	$3^-$	0.02985	-0.0346	0.03377	0.07385	0.03182	0.00132
3	0.8	$2^-$	0.79865	0.69725	0.78108	0.80051	0.79120	0.71581
4	0.892	$5^-$	0.88794	0.90249	0.75174	0.88318	0.65294	0.71776
5	2.1043	$1^-$	2.15004	2.02948	1.95270	2.07357	1.94711	1.88828
6	2.626	$0^-$	2.60825	2.62280	2.70511	2.83655	2.86116	2.92598
7	2.0473	$2^-$	2.08152	2.16279	1.78452	1.91236	2.30131	2.36065
8	2.0693	$3^-$	2.07096	1.98059	2.41998	2.47890	2.29364	2.35687
9	2.4575	$3^-$	3.91067	4.15917	2.54247	2.83730	2.79833	2.96056
10	2.3976	$4^-$	4.28711	4.31622	4.56933	4.83220	4.17144	4.30107
11		$1^-$	7.15585	7.30552	3.09319	3.23519	3.28519	3.47365
12		$2^-$	5.16547	5.22926	4.85632	5.10337	4.59455	4.80505
$\chi^2$			0.00171	0.46691	0.12955	0.17353	0.15297	0.31725

with effective potentials of the forms central, central + spin-orbit, central + tensor and central + spin - orbit + tensor are tabulated in Tables 3.7 - 3.10 respectively. The results quoted for pure central potential are those for the  $(\lambda_0, \lambda_1)$  set (0.38, 1.14) i.e. the one that gives an overall agreement with experimental spectrum.

It is clearly seen from the Tables 3.5 and 3.6 that addition of tensor force substantially worsens the value of  $\chi^2$  for levels predicted under the assumption of pure configurations. The energy of  $3_1^-$  state is 0.0296 MeV and, therefore, even small deviations in this level energy contribute largely to  $\chi^2$ . The largest effect that configuration mixing does to this nucleus is to reverse the ordering of  $4_1^-$  and  $3_1^-$  levels thus predicting the  $3_1^-$  level to be the ground state which is not true. It is because of this factor that  $\chi^2$  becomes much worse on diagonalization. It is only on the addition of the tensor force that the correct ordering of the  $4_1^-$  and  $3_1^-$  levels is achieved and the value of  $\chi^2$  for configuration mixed levels is also the best for the central + tensor form. In view of this it can be said that presence of tensor force is a must as a part of effective interaction for this

TABLE 3.7

Components in the wave-functions for different  
levels fitted with central force.

Predicted excitation energy (MeV)	$J^\pi$	$0d_{3/2}^{-1} 0f_{7/2}$	$0d_{3/2}^{-1} 1p_{3/2}$	$1s_{1/2}^{-1} 0f_{7/2}$	$1s_{1/2}^{-1} 1p_{3/2}$
2.14804	$1^-$		0.99371		0.11197
6.03039	$1^-$		0.11197		-0.99371
0.72310	$2^-$	-0.97716	0.18853		0.09801
2.01898	$2^-$	0.18011	0.97963		-0.08876
4.99446	$2^-$	0.11275	0.06908		0.99122
-0.04488	$3^-$	0.98695	-0.10762	0.11975	
2.68478	$3^-$	0.04635	0.90223	0.42876	
3.78248	$3^-$	0.15419	0.41762	-0.89545	
0	$4^-$	0.07335		0.99731	
4.37134	$4^-$	-0.99731		0.07335	

TABLE 3.8

Components in the wave functions for different levels fitted for central + spin - orbit form of the effective potential.

Predicted excitation energy (MeV)	$J^\pi$	$Od_{\frac{3}{2}}^{-1} \quad Of_{\frac{7}{2}}$	$Od_{\frac{3}{2}}^{-1} \quad 1p_{\frac{3}{2}}$	$1s_{\frac{1}{2}}^{-1} \quad Of_{\frac{7}{2}}$	$1s_{\frac{1}{2}}^{-1} \quad 1p_{\frac{3}{2}}$
2.02948	$1^-$		0.98711		0.16003
7.30552	$1^-$		0.16003		-0.98711
0.69725	$2^-$	-0.96142	0.27503		0.00606
2.16279	$2^-$	0.27208	0.95392		-0.12650
5.22926	$2^-$	0.04058	0.11997		0.99195
-0.08460	$3^-$	-0.97435	0.22200	-0.03680	
1.93059	$3^-$	-0.19856	-0.92511	-0.32364	
4.15917	$3^-$	0.10589	0.30804	-0.94546	
0	$4^-$	-0.99831		0.05807	
4.31622	$4^-$	0.05807		0.99831	



TABLE 3.9

Components in the wave functions for different levels fitted for central + tensor form of the effective potential.

Predicted excitation energy (MeV)	$J^\pi$	$0d_{\frac{3}{2}}^{-1} 0f_{\frac{7}{2}}$	$0d_{\frac{3}{2}}^{-1} 1p_{\frac{3}{2}}$	$1s_{\frac{1}{2}}^{-1} 0f_{\frac{7}{2}}$	$1s_{\frac{1}{2}}^{-1} 1p_{3/2}$
2.07357	$1^-$		-0.9954		0.0954
3.23519	$1^-$		0.0954		0.9954
0.80051	$2^-$	-0.9704	0.1946		0.1433
1.91236	$2^-$	0.2089	0.9736		0.0925
5.10337	$2^-$	0.1215	-0.1197		0.9854
0.07385	$3^-$	0.9833	-0.1291	0.1286	
2.47890	$3^-$	0.0324	0.9183	0.5739	
2.83780	$3^-$	0.1793	0.5601	-0.8088	
0	$4^-$	-0.9863		0.1649	
4.83220	$4^-$	0.1649		0.9863	

TABLE 3.10

Components in the wave function for different  
levels fitted for central + spin - orbit + tensor form  
of the effective potential.

Predicted excitation energy (MeV)	$J^\pi$	$Od_{\frac{3}{2}}^{-1}$ $Of_{\frac{7}{2}}$	$Od_{\frac{3}{2}}^{-1}$ $1p_{\frac{3}{2}}$	$1s_{\frac{1}{2}}^{-1}$ $Of_{\frac{7}{2}}$	$1s_{\frac{1}{2}}^{-1}$ $1p_{\frac{3}{2}}$
1.8828	$1^-$		-0.9602		0.2793
3.47365	$1^-$		0.2793		0.9602
0.71581	$2^-$	-0.9821	0.0355		0.1851
2.36065	$2^-$	0.0452	0.9978		0.0431
4.80505	$2^-$	0.1829	-0.0556		0.9816
0.00132	$3^-$	0.9835	-0.0341	0.1776	
2.35687	$3^-$	0.0485	0.9958	-0.0774	
2.96056	$3^-$	0.1742	-0.0847	-0.9811	
0	$4^-$	-0.9924		0.1228	
4.30107	$4^-$	0.1228		0.9924	

nucleus, to get correct ordering of the  $Od_{3/2}^{-1}$   $Of_{7/2}$  configuration levels at least, although correct excitation energy of the  $3_1^-$  level is not reproducible.

It can be seen that the spin-orbit and tensor forces act in opposite directions for the  $3_1^-$  level. Addition of spin-orbit to the central part further lowers the  $3_1^-$  level. On the other hand, addition of tensor part to the central part pushes up this level to the extent that correct ordering of the  $4_1^-$  and  $3_1^-$  levels is achieved with the  $3_1^-$  level appearing at 0.07385 MeV. Addition of both spin-orbit and tensor parts to the central part causes an elevation in the  $3_1^-$  level position, from a value obtained otherwise with the pure central force, which is much smaller than that obtained with the central + tensor form. Thus, with the central + spin-orbit + tensor form, the  $3_1^-$  level is predicted only at 0.00132 MeV and the overall agreement with experimental spectrum is also worst for this form. The discrepancy may largely be attributed to the fact that the  $3_3^-$  level at 2.4575 MeV had to be considered for determination of parameters and its appearance at a comparatively low energy makes the comparison of the matrix element

$$\langle 1s_{1/2}^{-1} Of_{7/2} 3_1^- | V_{\text{eff}} | 1s_{1/2}^{-1} Of_{7/2} 3_1^- \rangle$$

itself with the experimental energy doubtful.

It is anticipated that the  $3^-$  levels involve a substantial amount of configuration mixing (as judged from experimental level energies and single particle energies being used) due to which it should not be a valid assumption that the theoretical excitation energies, as calculated from unperturbed single particle energies and diagonal matrix elements of interaction, be directly equated to the experimental excitation energies. This is best illustrated by studying the wave functions for the  $3^-$  states as obtained with the central + tensor effective potential. The  $3_1^-$  level is relatively pure but the  $3_2^-$  and  $3_3^-$  levels are strongly mixed with each other. Such large configuration mixing is observed in none of the other levels. Since the effective potential of the form central + spin-orbit + tensor has been parametrized under the assumption of pure configuration for the  $3_3^-$  level, therefore the wave function for the  $3_3^-$  level is more pure in respect of the  $1s_{1/2}^{-1} 0f_{7/2}$  configuration than the corresponding structure for the effective potential of the form central + tensor. However, the  $3_3^-$  level for the central + spin - orbit + tensor effective potential is in worse agreement with experiment than the  $3_3^-$  level obtained with the central + tensor effective potential and we have seen that the spectrum is also overall worst reproduced in former case.

Energy levels of  $^{38}\text{Cl}$  as calculated with different effective potentials as determined for  $^{40}\text{K}$  are presented in Table 3.11. The results quoted for central effective potential are those obtained for the  $(\lambda_0, \lambda_1)$  set (0.38, 1.14). It is clearly seen that the  $3^-$  level position is in worst agreement - the effective potential of any form predicts  $3^-$  as the ground state  $J^\pi$  instead of  $2^-$  as experimentally observed. The  $3^-$  predicted level is closest to zero for the effective potential of the form central + spin-orbit. However, we may recall that this potential was also the one which gave the worst agreement for  $3_1^-$  level in  $^{40}\text{K}$ . The central + tensor potential predicted correct ordering of  $4_1^-$  and  $3_1^-$  levels in  $^{40}\text{K}$  but for  $^{38}\text{Cl}$ , this form predicts a deepest  $3^-$  level. These observations regarding the behaviour of  $3^-$  levels are in ~~in~~confirmity with those of Fink and Schiffer<sup>139</sup> who find that an improved value of  $(\text{Od}_{3/2} \text{ Of}_{7/2})$  two-particle matrix element in  $^{38}\text{Cl}$  predicts a worse agreement for  $3^-$  level in  $^{40}\text{K}$ . However, except for the  $3^-$  level, the ordering of the lowest  $2^-$ ,  $5^-$  and  $4^-$  levels is correctly reproduced and the excitation energies of  $5^-$  and  $4^-$  levels are in quite an impressive agreement with corresponding experimental numbers. Nothing much should be expected of the form central + spin-orbit + tensor for reasons discussed above. However, the form central + tensor

TABLE 3.11

Level excitation energies of  $^{38}\text{Cl}$  predicted for different forms of the effective potential with parameters as those given in Table 3.4. For any form of the potential, set I of levels is for pure particle-particle configurations and set II gives level energies on diagonalization. To facilitate comparison with experiment, all excitation energies have been calculated relative to the  $2_1^-$  level.

Expt. (MeV)	$J^\pi$	Central		Central + spin-orbit	
		I (MeV)	II (MeV)	I (MeV)	II (MeV)
0	$2^-$	0	0	0	0
0.67127	$5^-$	0.69494	0.71470	0.69512	0.72939
0.75526	$3^-$	-2.72652	-2.78045	-0.83476	-0.81810
1.30887	$4^-$	1.32250	1.34226	1.32177	1.35604
	$0^-$	-0.08350	-0.06375	1.11642	1.15069
	$1^-$	2.10979	2.12955	3.08537	3.11964
	$2^-$	2.96838	2.90790	3.05396	3.12250
	$3^-$	0.30610	0.39955	1.41411	1.46599

Contd. Table 3.11

Contd. Table 3.11

Expt. (MeV)	$J^\pi$	Central + tensor		Central+spin-orbit+tensor	
		I	II	I	II
0.0000	$2^-$	0	0	0	0
0.67127	$5^-$	0.51963	0.54318	0.37851	0.37966
0.75526	$3^-$	-6.64042	-7.05091	-5.73825	-6.32996
1.30887	$4^-$	1.14031	1.16386	1.01757	1.01882
	$0^-$	1.46004	1.48359	-0.85892	-0.85767
	$1^-$	0.09179	0.11534	0.23312	0.23437
	$2^-$	3.02191	3.06905	2.58219	2.58469
	$3^-$	0.51689	0.98048	-0.11107	0.48314

also does not reproduce the excitation energy of the  $5^-$  level as well as is done by central and central + spin-orbit forms. Best agreement, excepting the  $3^-$  level, with experimental spectrum is found with the central effective potential.

#### III.4 CONCLUSIONS:

Above discussion makes it clear that for the problem of  $^{40}\text{K}$  and  $^{38}\text{Cl}$  nuclei, it is possible to parametrize effective potentials for the  $^{40}\text{K}$  nucleus in such a way that besides those of  $^{40}\text{K}$ , energy levels of  $^{38}\text{Cl}$  are also satisfactorily reproduced. The maximum discrepancy is observed in  $3^-$  levels. The tensor force plays an important role in  $^{40}\text{K}$  nucleus particularly for the  $3_1^-$  level. The level energies in  $^{40}\text{K}$  and  $^{38}\text{Cl}$  are correlated in such a way that an improvement in levels of  $^{40}\text{K}$  causes those of  $^{38}\text{Cl}$  to become worse. The results are worst for the form central + spin - orbit + tensor, the possible reason for which has also been discussed above. In view of this it can be said that the parameters of the effective potential of the form central + spin - orbit + tensor are a forcible imposition of mathematics on physics - the oldest question on validity of parameters of a phenomenological effective interaction.



feeling that nuclear level energies are relatively insensitive to details of effective interaction - closed shell + two nucleons nuclei are the most widely studied ones and it has often been found that two different forms of effective interaction give almost equally good fit to level spectra. However, the wave functions do depend upon the details of effective interaction. Energy levels arise as an interplay between effective interaction and the wave functions (which have been derived by diagonalizing the matrix of effective Hamiltonian!) Therefore, it is believed that other properties of levels, e.g. their electromagnetic properties, provide a sensitive test to the real 'goodness' of an effective interaction. Surprisingly though, they observed that 'pseudo-experimental' data on level properties, even the electromagnetic properties of nuclei  $^{41}\text{Pb}$  to  $^{48}\text{Pb}$  were excellently reproduced by assuming an effective interaction and pure  $(f_{7/2})^{N-4}$  configuration. Their results also simultaneously proved the non-uniqueness of effective interaction. It was observed that the effective interaction could be obtained either as a mixture of central, spin-orbit and tensor components or as a superposition of an additional pairing force over the original potential, however, whose both the  $S = 0$  and  $S = 1$  strengths are multiplied by the same factor  $\alpha (> 1)$ .

Thus, the two effective interactions differed not only in effective potential parameters but also in the phenomenology adopted for the choice of effective potential.

Were it not for the strong configuration mixing involved (50 per cent or more), results of Cohen et.al. were also one among those obtained by so many others who try to parametrize effective interaction for explaining experimental data. After all, an effective interaction is designed to reproduce experimental data in a model space. The fact that such large configuration mixing as occurred in their calculations could also be concealed in the effective interaction parameters was surprising.

In a problem like that of nuclear structure physics we can atmost establish an effective interaction and say that it is the nature of the N-N force - of course, in the particular model space chosen. Otherwise, in a different model space we might arrive at a different effective interaction and so on. Therefore, it was felt that if the results of Cohen et.al. could be shown to be true in different mass regions, it would very much reduce computational troubles since one could then take just the lowest  $j^n$  configuration or a small number of low-lying configurations as the model space and

parameterize the energy levels in this model space. With these points in mind, Gupta and Trainor<sup>17</sup> and Engel and Unna<sup>143</sup> did similar calculations for sd-shell and fp-shell configurations and found that results of Cohen et.al. did not have generality over different sets of configurations and that nuclear properties dependant on wave functions could still provide a sensitive test of true effective interaction.

While these conclusions may be somewhat academic since they are drawn from models involving only two subshells, they probably suggest a lesson for any study using a truncated configuration space.

In light of these observations let us discuss again some of our results for the  $^{92}\text{Zr}$  as obtained in Chapter II. Let us consider only the central part of the SME and analyse the structure of  $O_3^+$  level. We have seen that the dominant configuration contributing to this level for set II and set III of single particle energies is just different from the one which makes up most of the  $O_3^+$  level with set I of single particle energies. With set I, the  $O_3^+$  level receives dominant contribution from  $(1d_{3/2})^2$  configuration whereas with both set II and set III, the  $(0g_{7/2})^2$  configuration contributes most to the  $O_3^+$  level. In practice, one will

use the total interaction rather than just the central part. However, it should be recalled that we had used set II with the reasoning that single particle spectrum of  $^{89}\text{Sr}$  can also be used for  $^{91}\text{Zr}$  whereas set III was given by Cohen<sup>128</sup> specifically for  $^{91}\text{Zr}$  nucleus. Therefore, if we consider only set I and set III

	Set I (MeV)	Set III (MeV)
$1d_{5/2}$	0	0
$2s_{1/2}$	1.22	1.55
$1d_{3/2}$	2.07	2.70
$0g_{7/2}$		2.70

we see that for both the total interaction and its central part the predicted structure of the  $0_3^+$  level so crucially depends on space dimensionality and single particle energies being used whereas the energy of this level as calculated with bare SME with set I and set III turns out to be 3.77369 MeV and 4.39721 MeV respectively. The two energy values are of the same order of magnitude. Suppose we can locate the  $0_3^+$  level in spectrum of  $^{92}\text{Zr}$ .

Further, let us assume we are able to make a best possible renormalization of bare interaction. Unless we can be definite to say, there is no a priori reason to believe that each of these two energies will not be close enough to the experimental energy level. Further assuming that the renormalization process does not change the basic structure of a wave function - as regards the relative dominance of main contributor configuration, we thus find that like this there can exist more than one wave function - each of them being drastically different in structure from the other such that each of them gives satisfactory reproduction of experimental energies. We realize that such a situation arises because relative to set I, set III contains one more configuration in the model space.

What we have said is speculation on our part on the basis of assumption that the renormalization process does not change the basic structure of a wave function. It might also happen the other way that on renormalization, the  $0_3^+$  level calculated with set III also receives dominant contribution from  $(1d_{3/2})^2$  configuration.

Our experience with microscopic calculations tells that every other day we have been discovering a new renormalization process and unless a consistent theory

is available, above doubts cannot be checked but they certainly raise a more fundamental question - how to properly choose a model space? We observed the particular behaviour of the  $O_{3/2}^+$  level of  $^{92}\text{Zr}$  for set III of single particle energies and a model space of four configurations. In each of the model spaces we might find a satisfactory effective interaction where the effectiveness is brought to take into account the effect of neglected configurations. However, not much faith should be put in an effective interaction which brings about fundamental changes in the structure of wave functions - it sounds reasonable to absorb effects of neglected configurations through effectiveness only so long as they are small. For example, for spectrum of  $^{92}\text{Zr}$  it appears that one cannot do without including the  $O_{3/2}$  configuration in model space.

Therefore, before one starts out for an ambitious programme of nuclear structure calculations, the dispute over the model space to be worked in should be settled. At present there does not exist any specific prescription as to which configurations should be included in diagonalization. Practice, adopted by almost everybody, till now has been to choose the model space as encompassing the major shell, the lowest partially filled orbit of which is occupied by the valence nucleons. In case of

phenomenological effective interactions, the effect of neglected configurations is forced to be absorbed in parameters. In case of effective interactions derived from realistic interactions, these effects are calculated in perturbation theory, though lately it has also been realized that the configurations which have hitherto been treated in perturbation theory should better be included directly in diagonalization to understand a truer picture of effective interaction. Lo Iudice et.al.<sup>70,71</sup> have made such calculations.

With this question in mind we undertake the present study. In philosophy, our study is not very much different from earlier works on pseudo-nuclei. However, instead of pseudo-nuclei we take just one nucleus -  $^{42}\text{Sc}$ . It has a proton and a neutron in  $0f_{7/2}$  orbit. This gives us a chance to study all the four spin-isospin components of a central interaction. The model space generally chosen for this nucleus is full fp - shell where single particle energies are:

	Single particle energy (MeV)
$0f_{7/2}$	0
$1p_{3/2}$	2.0
$1p_{1/2}$	4.0
$0f_{5/2}$	6.45

This is also a favourable situation that there are four configurations in fp-shell so that the effect of gradually expanding the model space can be better investigated in four spaces. The similar case can also be of sdg - shell but in the mass region (4-90), where valence nucleons are in one of the orbits of sdg-shell, it is not possible to find a self-conjugate nucleus where both neutron and proton might be in same orbit in ground state so that both isospin components might be studied. Further, these nuclei have neutron excess so that even if we picked up a nucleus where odd neutron and odd proton were in different orbits, the states will not have good isospin which will, hence, be projected. Above all, calculations are much more lengthy in higher mass region. Furthermore, the highest configuration contributing in fp-shell is  $(Of_{5/2})^2$  with unperturbed energy 12.9 MeV which does not occur in any of lower major shell, sdg-shell and also not expected to occur in still higher mass region where single particle levels are more closely spaced. The unperturbed energy  $\sim 13$  MeV configuration is believed to be weak enough in contribution as regards its effect on low-lying levels. Therefore, if the effect on low-lying levels of expanding the space from  $(Of_{7/2}, 1p_{3/2}, 1p_{1/2})$  to  $(Of_{7/2}, 1p_{3/2}, 1p_{1/2}, Of_{5/2})$  can be shown to be substantial, it will be



indicative of nonconvergence of effective interaction as regards space dimensionality. Since, then it will be no guarantee that configurations lying above the  $0f_{5/2}$  level really have a small effect.

We arbitrarily choose the parameters of a central two-nucleon potential with the only presumption that the level energies calculated with them do not turn out to be orders of magnitude off the experimental numbers so that qualitative results which we would be concluding afterwards do not turn out to be completely hypothetical. Then, keeping them within limits as allowable in this sense, we study levels arising from the  $(0f_{7/2})^2$  configuration as a function of interaction parameters and space dimensionality.

#### IV.2 METHOD OF CALCULATION:

The  $(0f_{7/2})^2$  configuration gives rise to following levels:

$$T = 0 : \quad 1^+, \quad 3^+, \quad 5^+, \quad 7^+$$

$$T = 1 : \quad 0^+, \quad 2^+, \quad 4^+, \quad 6^+$$

We assume a central two-body potential of the form

$$V_C(r) = \sum_{T,S} {}^{2T+1,2S+1}P \Lambda_{TS} \frac{e^{-(r/r_0)}}{(r/r_0)}$$

where  ${}^{2T+1, 2S+1}P$  is the projection operator which projects out two-nucleon states of isospin  $T$  and spin  $S$  and  $\Lambda_{TS}$  is strength in the  $(T,S)$  channel. We define

$$\lambda = \frac{r_0}{\sqrt{2}b}$$

and

$$P = \left( \frac{\lambda^2}{1+\lambda^2} \right)^{1/2}$$

and set

$$P = 0.5$$

which corresponds to  $\lambda = 0.57735$  which, in turn, corresponds to  $r_0 = 1.6328$  fm which is acceptable as range of two-nucleon force.

The two-body matrix elements, for a given set of  $\Lambda_{TS}$  values are calculated using eq. (A.30) as given in appendix A where the relative matrix elements are calculated in terms of Talmi integrals  $I_p$ 's and the coefficients  $B(nl, n'l', p)$ . The coefficients  $B(nl, n'l', p)$  are taken from ref. 144 and Talmi integrals for

Yukawa shape are calculated for the chosen value of  $\lambda$  using

$$I_0 = v_0 \lambda \left[ \frac{2}{\sqrt{\pi}} - 2\mu(1-\phi(\mu)) e^{\mu^2} \right]$$

$$I_1 = \frac{2}{3} v_0 \lambda \left[ \frac{2}{\sqrt{\pi}} (1+\mu^2) - 2\mu \left( \frac{3}{2} + \mu^2 \right) (1-\phi(\mu)) e^{\mu^2} \right]$$

$$I_{p+1} = \frac{2p}{2p+3} \left[ \left( 2 + \frac{2\mu^2+3}{2p} \right) I_p - I_{p-1} \right]$$

where,

$$\mu = \frac{1}{2\lambda}$$

and

$$\phi(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt$$

are error functions tabulated in ref. 145.

The odd -  $\ell$  states are believed to contribute weakly in comparison to even- $\ell$  ones. With this realization, people have also often succeeded in establishing phenomenological effective interactions which act in even  $\ell$  states only (Serber force) or even in just relative S-states. Including the odd  $\ell$  relative states just for the sake of inclusion adds at least one more parameter. Therefore, if in a problem it can be shown that odd  $\ell$  states really contribute much less than even  $\ell$  ones it might as well be a good approximation to

altogether drop this part of the interaction. Similarly, it may also be possible that some of the configurations within the conventionally chosen model space affect the level energies very little. We, therefore, study levels arising from the  $(Of_{7/2})^2$  configuration as a function of all the four  $A_{TS}$  parameters in different model spaces. In such a study, the points raised just now can be investigated. If the points can be established, it will be reasonable to drop the less effect producing interaction parameters and model space configurations so as to make place for other more important effects. This has to be done in view of the reality that only rather limited amount of experimental information is available for parametrization of effective interaction and hence best use should be made of it.

For the nature of above study, we should individually investigate all the eight levels of the  $(Of_{7/2})^2$  configuration as a function of the various parameters. However, to facilitate analysis, we study the splitting between centroids of  $T = 1$  and  $T = 0$  levels of the  $(Of_{7/2})^2$  configuration

$$\Delta E = \bar{E}_1 - \bar{E}_0$$

where 
$$\bar{E}_T = \frac{\sum_J (2J+1) E_{J,T}}{\sum_J (2J+1)}$$

For the  $(0f_{7/2})^2$  configuration, J and T are related through

$$J + T = \text{Odd}$$

and  $E_{J,T}$  is the energy of the particular (J,T) state.

The exact calculational details are as follows: Suppose we are studying the effect of variation of T=0 strength parameters  $\lambda_{0S}$ . Then we fix:

$$\lambda_{10} = -40 \text{ MeV} \quad \text{and} \quad \lambda_{11} = -50 \text{ MeV}.$$

Further, when we are studying the effect of  $\lambda_{01}$  component on spectra to assess its relative importance we fix  $\lambda_{00} = -70 \text{ MeV}$  and let  $\lambda_{01}$  vary between -40 MeV and -80 MeV in steps of 10 MeV. At each of these parameters sets we calculate energy levels arising predominantly from the  $(0f_{7/2})^2$  configuration and thence  $\Delta E$ . It can be realized that within a fixed model space, if only T = 0 interaction is being varied, the T = 1 centroid will stay at a constant level and vice versa. After these five runs, to study effect of  $\lambda_{00}$  component

We fix  $\Lambda_{01} = -70$  MeV and let  $\Lambda_{00}$  vary between  $-40$  MeV and  $-80$  MeV as above. After this is complete we fix:

$$\Lambda_{00} = -40 \text{ MeV} \quad \text{and} \quad \Lambda_{01} = -50 \text{ MeV}$$

and vary the  $\Lambda_{1S}$  parameters on exactly same range of values as for  $\Lambda_{0S}$  parameters. Like this when variation of all the four strength parameters is studied we repeat these calculations in a different model space using the same values of strength parameters. Thus, we study the effect of configuration mixing on each of the lowest eight levels of  $J^\pi = 0^+, 1^+, 2^+, 3^+, 4^+, 5^+, 6^+$  and  $7^+$  which are expected to arise predominantly from the  $(0f_{7/2})^2$  configuration.

The general nature of the two two-nucleon interaction can also be discussed from behaviour of  $\Delta E$  with respect to the various parameters. However, some typical behaviour of  $\Delta E$  can be subanalyzed in terms of behaviour of individual energy levels.

We have said that when variation of  $\Delta E$  in a given space with respect to one isospin component is being studied, the centroid of the other isospin levels stays stationary and is, thus, redundant. However, study of  $\Delta E$  at a given  $\Lambda_{TS}$  set in different spaces is

expected to reveal the relative behaviour of the two isospin components in the different spaces e.g. if on expanding the space, the splitting  $\Delta E$  increases, centroids of both  $T = 0$  and  $T = 1$  levels will no doubt go down, this would mean that the centroid of  $T = 0$  states is lowered more than that of  $T = 1$  states i.e. the new added configuration affects the  $T = 0$  levels more than  $T = 1$  ones.

Within fp-shell, biggest matrices occur for  $2^+$  and  $3^+$  states - each of dimensionality eight. We have made exact diagonalization for calculations within fp-shell. However, for later part of the calculation where we include still higher configurations, we do not make exact diagonalization. Instead, we calculate the effect of added configuration in an approximate way as follows:

For a  $2 \times 2$  Hamiltonian matrix

$$\begin{pmatrix} H_{11} & H_{12} \\ H_{12} & H_{22} \end{pmatrix}$$

assuming  $H_{11} < H_{22}$ , the lower perturbed energy is

$$\lambda = \frac{(H_{11} + H_{22}) - \sqrt{(H_{11} - H_{22})^2 + 4 H_{12}^2}}{2}$$

Thus, the effect of perturbation i.e. the off-diagonal matrix element on  $H_{11}$  is

$$H_{11} - \lambda = \frac{H_{12}^2}{|H_{11} - H_{22}|} - \frac{H_{12}^4}{|H_{11} - H_{22}|^3} + \dots$$

Therefore, if the off-diagonal matrix element is small and the separation between the two diagonal matrix elements quite large, approximately

$$H_{11} - \lambda \simeq \frac{H_{12}^2}{|H_{11} - H_{22}|}$$

or

$$\lambda \simeq H_{11} - \frac{H_{12}^2}{|H_{11} - H_{22}|}$$

Thus, the effect of exact diagonalization can be approximately treated through calculation of

$$\frac{H_{12}^2}{|H_{11} - H_{22}|} . \text{ For the problem of nuclear energies, the}$$

diagonal matrix elements contain the unperturbed excitation energy of the two-particle configuration and the diagonal matrix element of the two particle interaction in excited configuration. However, for a highly excited configuration, the denominator may be approximated by just the sum of single particle excitation energies of the excited configuration.



Such a simple derivation is not possible for a many-level system. However, to first approximation, the effect of diagonalization can be estimated by calculating the second-order contribution of each off-diagonal matrix element as above and, for a given matrix, adding all of them. Thus, due to configuration mixing arising from various two-particle configurations  $|j\rangle$ , the modified energy of a configuration  $|i\rangle$  is obtained through

$$\lambda_i = \langle i | V | i \rangle - \sum_{j \neq i} \frac{|\langle i | V | j \rangle|^2}{e_j}$$

where  $e_j$  is the appropriate approximate energy denominator for the configuration  $|j\rangle$  as discussed above.

In what follows we shall call  $\frac{|\langle i | V | j \rangle|^2}{e_j}$  the second-order contribution of configuration  $|j\rangle$  and denote it by  $S$ . For calculations within fp-shell,  $I_{nl}$ 's for all relative  $\ell$  states i.e. 0 to 6 were included. However, to make things speedier and easier in calculation, for calculation of inclusion of higher configurations, only  $\ell = 0, 1$  and  $2$  were considered. It had been checked that the effect of inclusion of higher partial waves would be additive only so that the second-order contributions as reported here will increase..

An idea of relative importance of relative states of  $\ell > 2$  can be had from an example. In the  $12^+$  state arising from  $(0i_{13/2})^2$  configuration, 12 percent of the total of the spin-singlet and 20 per cent of the total of the spin triplet contribution to the total matrix element comes from  $\ell > 2$  partial waves of the interaction. We have also made similar analysis for  $6^+$  levels arising within the fp-shell i.e. from the configurations  $(0f_{7/2})^2$  and  $(0f_{5/2} 0f_{7/2})$ . We assume  $A_{10} = -40$  MeV and  $A_{11} = -50$  MeV. The total matrix element for  $6^+$  state in the  $(0f_{7/2})^2$  configuration is  $-1.5422$  MeV out of which  $-0.2648$  MeV i.e. around 15 per cent comes from contribution of  $\ell > 2$  waves. The perturbed  $6^+$  level with inclusion of contribution of all  $\ell$  values is at  $-1.5747$  MeV and the splitting between the two  $6^+$  levels is  $5.6406$  MeV. Ignoring the contribution of  $\ell > 2$  waves, the perturbed  $6_1^+$  level is predicted at  $-1.32095$  MeV with a splitting of  $5.5378$  MeV between the two  $6^+$  levels.

#### IV.3 RESULTS AND DISCUSSION:

First of all we see the order of magnitude of level energies for a randomly chosen set of parameters. We choose

$$\Lambda_{10} = -40 \text{ MeV}$$

$$\Lambda_{11} = -50 \text{ MeV}$$

$$\Lambda_{00} = -70 \text{ MeV}$$

$$\Lambda_{01} = -60 \text{ MeV}$$

Then, for pure  $(0f_{7/2})^2$  configuration, excitation energies in respective sets of levels of the two isospins, relative to the lowest level of that isospin, are tabulated in Table 4.1. We see that even without any reservation towards strength parameters, the  $T = 1$  excitation spectrum resembles the experimental spectrum very much. The discrepancy is unignorable for  $T = 0$  spectrum. Similar situation was also encountered while working with Sussex matrix elements in Chapter II. However, our aim is not to do parameter fitting and except for the splitting of  $1^+$  and  $7^+$  levels, numbers for  $3^+$  and  $5^+$  levels are tolerable. For the same set of parameters we also calculate the excitation spectrum relative to the ground state  $0^+$  level. We present the comparison of predicted spectrum with experimental one in Table 4.2. Thus, except for inversion of  $0^+$  and  $1^+$  levels and of  $5^+$  and  $2^+$  levels, the level ordering is correctly reproduced.

TABLE 4.1

Excitation energies, calculated separately for  $T = 0$  and  $T = 1$  sets of levels, arising from pure  $(Of_{7/2})^2$  configuration for  $A_{10} = -40$  MeV,  $A_{11} = -50$  MeV,  $A_{00} = -70$  MeV,  $A_{01} = -60$  MeV. For comparison, experimental excitation energies are also given.

$J^\pi$	$T = 0$		$J^\pi$	$T = 1$	
	Calculated (MeV)	Experimental (MeV)		Calculated (MeV)	Experimental (MeV)
$1^+$	0	0	$0^+$	0	0
$7^+$	1.1346	0.007	$2^+$	1.8333	1.59
$3^+$	2.0548	0.879	$4^+$	2.6441	2.81
$5^+$	2.5899	0.899	$6^+$	2.8154	3.24

TABLE 4.2

Calculated excitation spectrum of levels  
 arising from  $(0f_{7/2})^2$  configuration for  $A_{10} = -40$  MeV,  
 $A_{11} = -50$  MeV,  $A_{00} = -70$  MeV and  $A_{01} = -60$  MeV.

$J^\pi$	Experimental (MeV)	Calculated (MeV)
$6^+$	3.24	2.8154
$4^+$	2.81	2.6441
$2^+$	1.59	1.8333
$5^+$	1.51	1.9257
$3^+$	1.49	1.3906
$7^+$	0.618	0.4704
$1^+$	0.611	-0.6642
$0^+$	0	0

It was checked that the ordering of  $2^+$  and  $5^+$  levels can be correctly reproduced by taking  $A_{01} = -63$  MeV instead of  $-60$  MeV, however, the  $0^+$  and  $1^+$  levels still remain inverted.

The results for  $\Delta E$  as a function of  $A_{00}$ ,  $A_{01}$ ,  $A_{10}$  and  $A_{11}$  are plotted in Figures 4.1 - 4.4 respectively. In each figure, results of calculation for the variation of that particular  $A_{TS}$  parameter in the four model spaces

I  $0f_{7/2}$

II  $0f_{7/2} \ 1p_{3/2}$

III  $0f_{7/2} \ 1p_{3/2} \ 1p_{1/2}$

IV  $0f_{7/2} \ 1p_{3/2} \ 1p_{1/2} \ 0f_{5/2}$

are shown.

In any of the spaces, when varied over same range of values,  $\Delta E$  is found to behave most sharply with  $A_{01}$ . A strange thing is observed to happen in Figure 4.2 for  $A_{01} = -80$  MeV. In all the spaces II, III and IV, configuration mixing increases fast with  $|A_{01}|$ . Upto  $A_{01} = -70$  MeV, the lowest levels of all J's of  $T = 0$

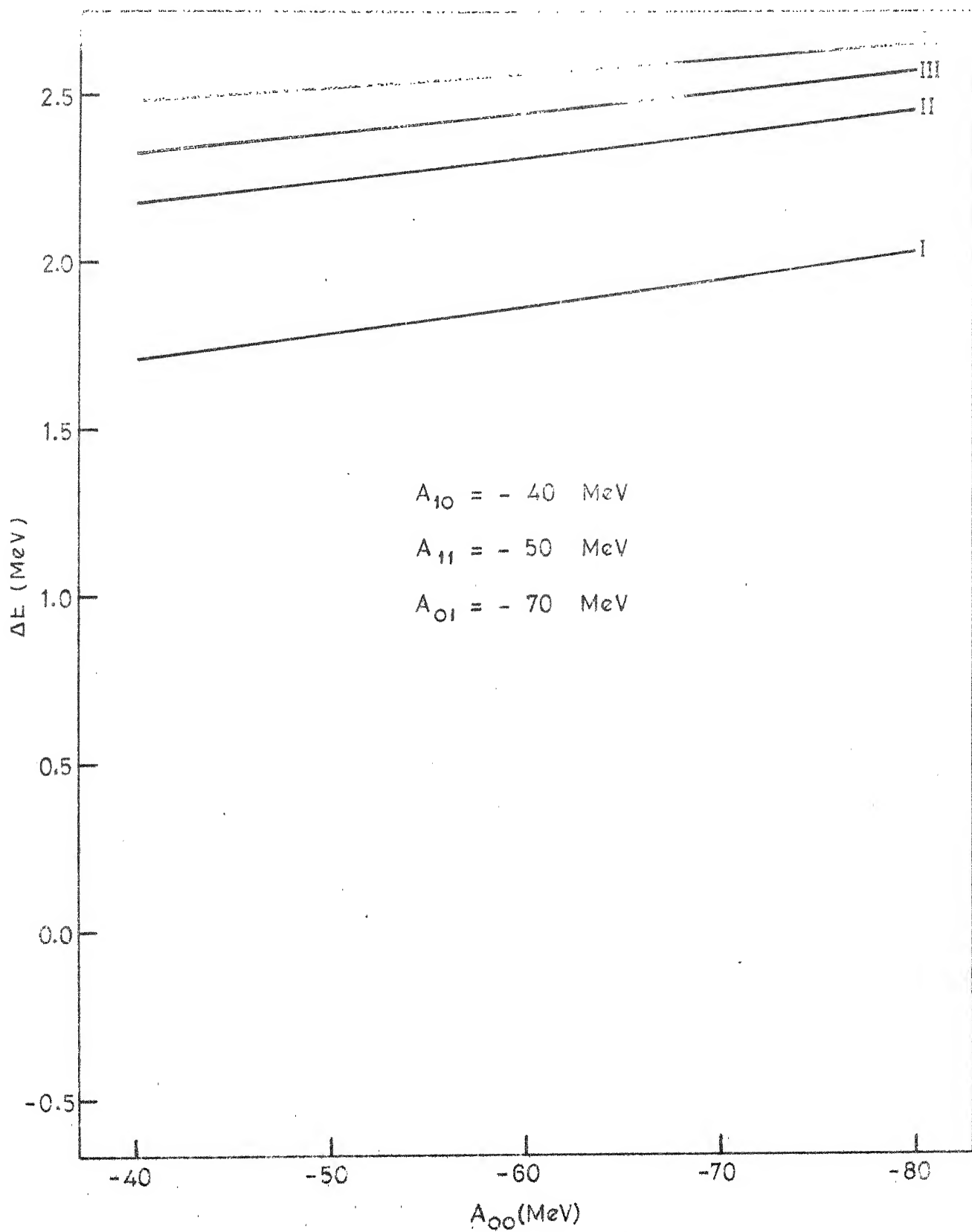


Fig. 4.1.  $\Delta E$  plotted as a function of  $A_{00}$  in different spaces (denoted by I, II, etc. see the text)

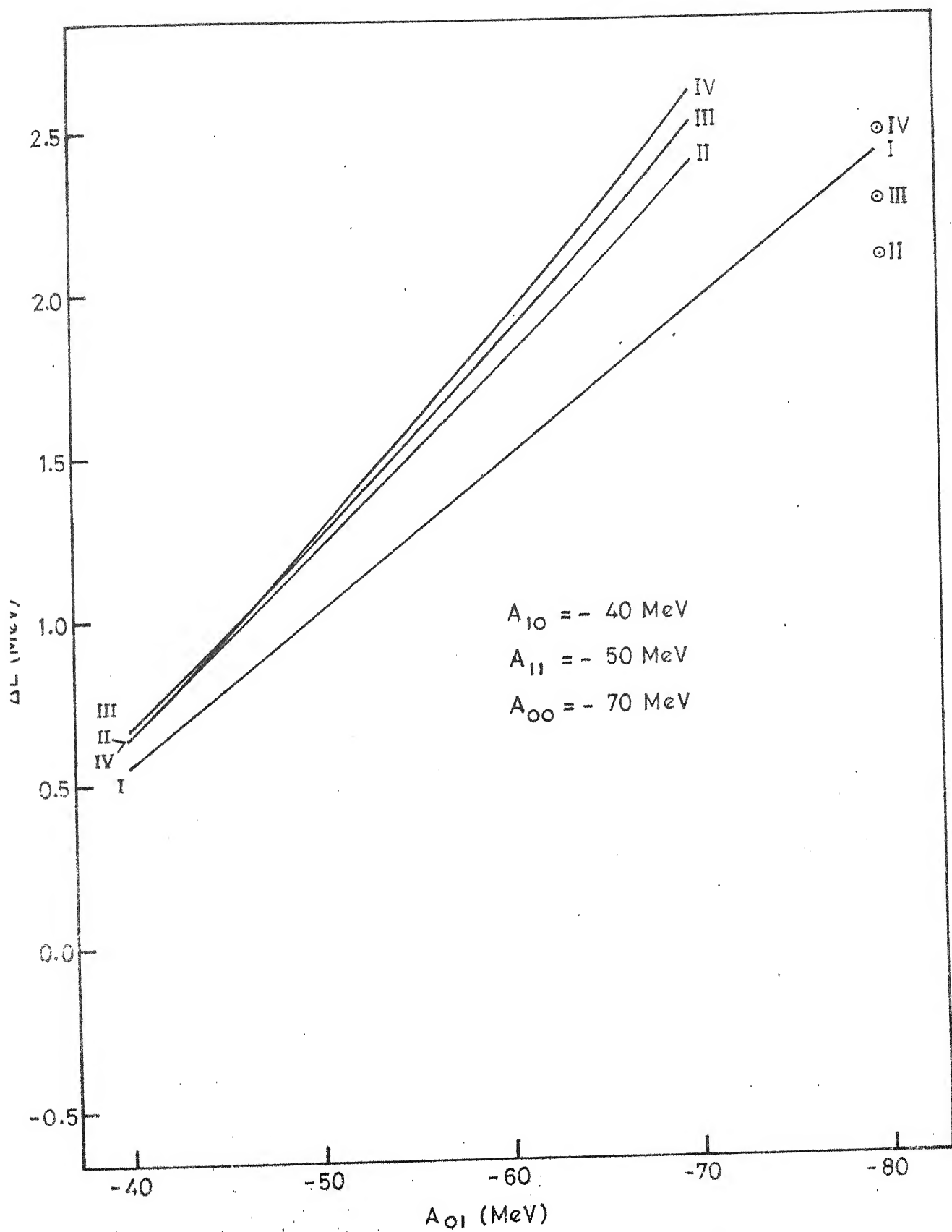


Fig. 4.2.  $\Delta E$  Plotted as a function of  $A_{0I}$  in different spaces



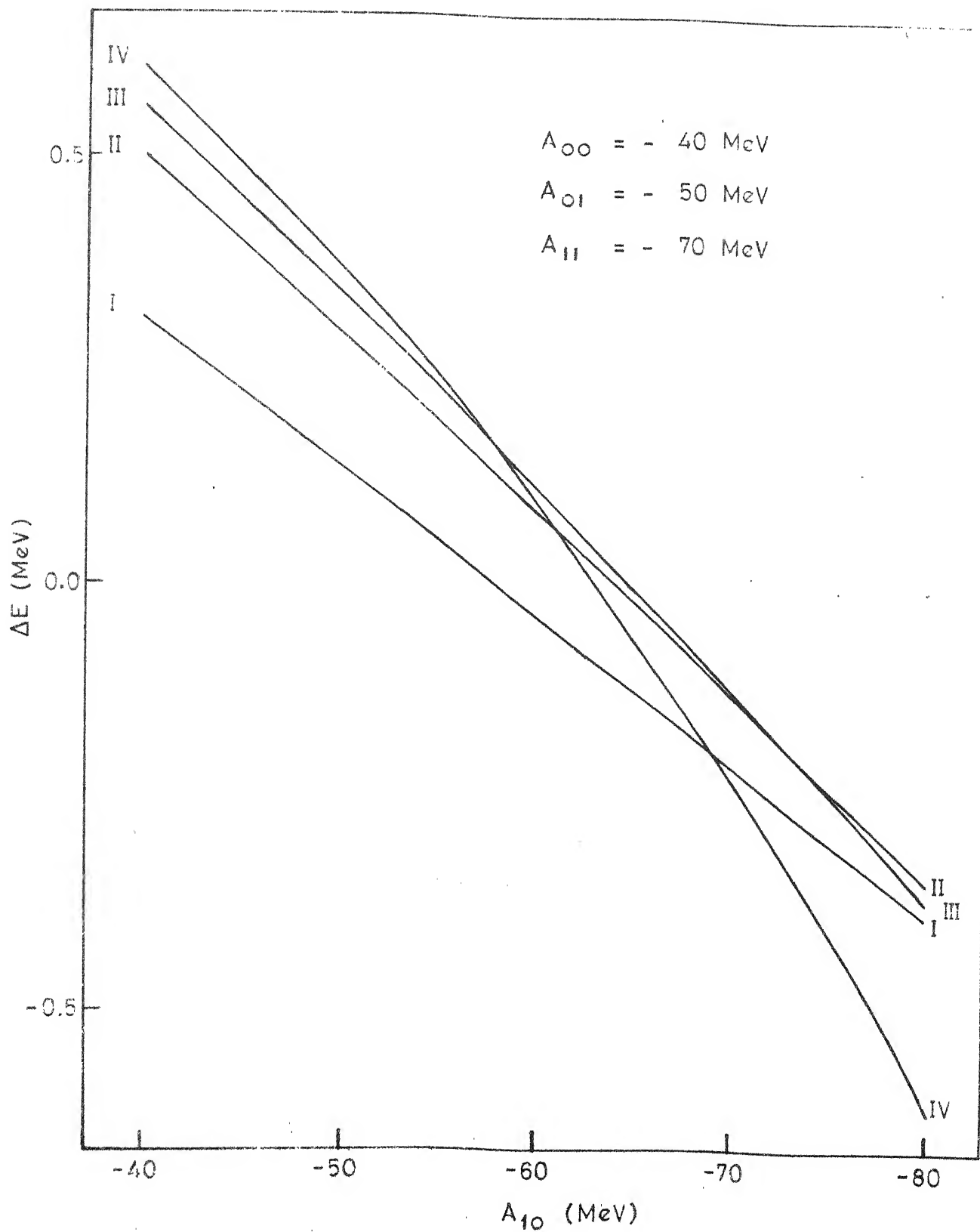


Fig. 4.3.  $\Delta E$  plotted as a function of  $A_{10}$  in different spaces

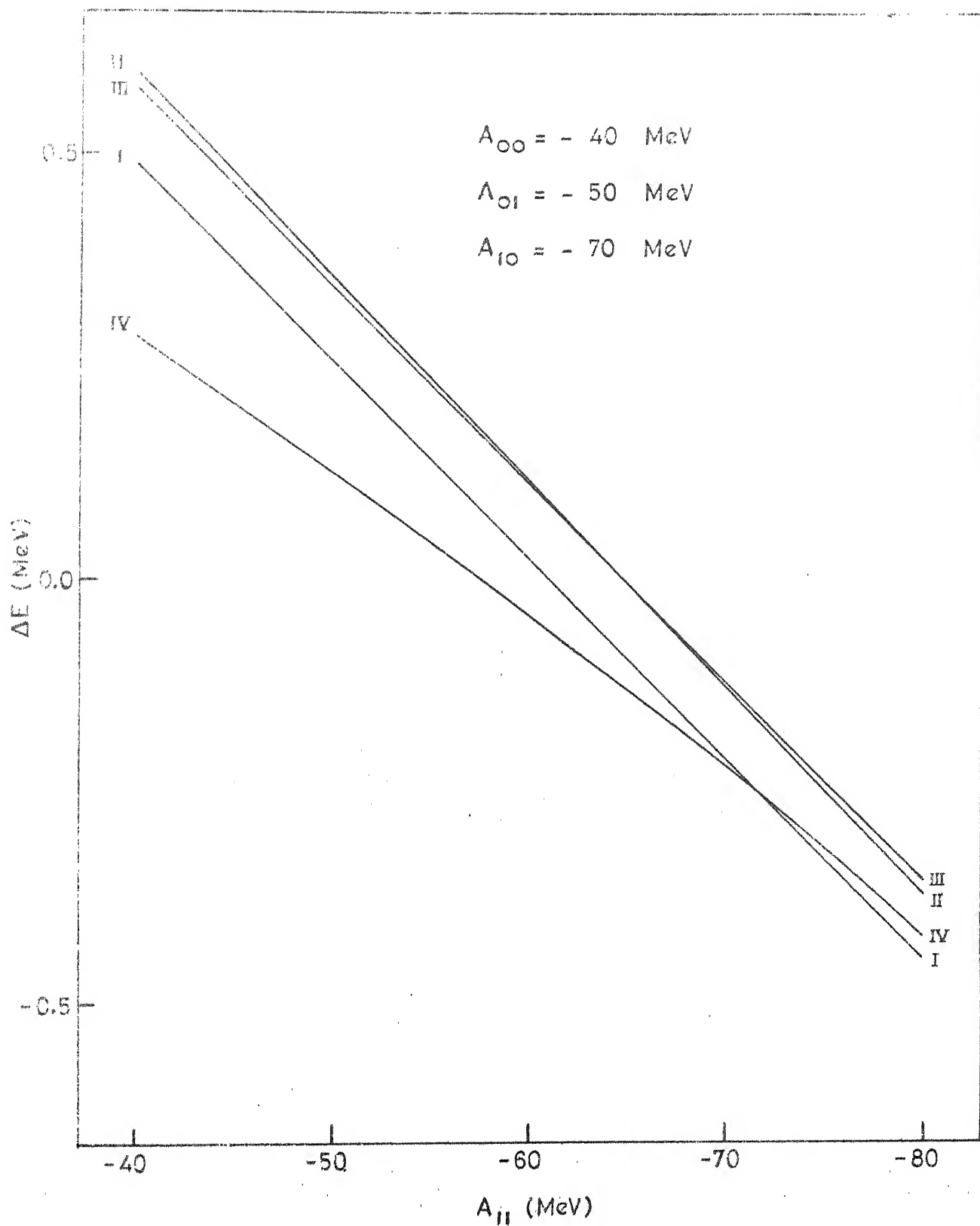


Fig.4.4.  $\Delta E$  plotted as a function of  $A_{11}$  in different spaces

can be identified as containing a predominant  $(Of_{7/2})^2$  component. However, for  $\Lambda_{01} = -80$  MeV, the  $1^+$ ,  $3^+$  and  $7^+$  levels still receiving dominant contribution from the  $(Of_{7/2})^2$  configuration, the  $5_1^+$  level receives dominant contribution from the  $(1p_{3/2} Of_{7/2})$  configuration and it is the  $5_2^+$  level which comes predominantly from the  $(Of_{7/2})^2$  configuration. This pushes up the centroid of the  $T=0$  levels because the  $5^+$  level occurs with a weight 11. Therefore, plotting a smooth curve between  $\Lambda_{01} = -70$  MeV and  $-80$  MeV only on the basis of extrapolation of graph between  $\Lambda_{01} = -40$  MeV and  $-70$  MeV and the value of  $\Delta E$  at  $\Lambda_{01} = -80$  MeV is not correct. In fact, it would require a point-to-point calculation of  $\Delta E$  in the region of  $\Lambda_{01}$  values between  $-70$  MeV and  $-80$  MeV. Comparison of graphs for variation of  $\Lambda_{00}$  and  $\Lambda_{01}$  strengths clearly demonstrates the relative importance of  $\Lambda_{01}$  parameter over  $\Lambda_{00}$ . In fact,  $\Delta E$  becomes more and more sharp function of  $\Lambda_{01}$  as the space is expanded and, opposite to it, mixing seems to smoothen the behaviour of  $\Delta E$  with  $\Lambda_{00}$ . In space IV, the change in value of  $\Delta E$  in going from  $\Lambda_{00} = -40$  MeV to  $\Lambda_{00} = -80$  MeV is about half the corresponding value in space I which itself is much smaller than the

variation in  $\Delta E$  in going from  $A_{01} = -40$  MeV to  $-80$  MeV even in space I. Therefore, it can be concluded that if it is planned to parametrize an effective interaction for the full fp-shell, it is quite safe to ignore the  $A_{00}$  part altogether i.e. consider a central interaction contributing to even  $\ell$  states only (i.e. a Serber force). However, the discussion here is restricted to comment only on the central part of effective interaction. Study of Figure 4.1 reveals that the  $T = 0$  interaction does not give saturation of  $\Delta E$  as regards space dimensionality within fp-shell. At larger  $|A_{01}|$  values, Figure 4.2 also reveals the same thing.

Behaviour of the interaction components  $|A_{1S}|$  in different spaces is more complicated than the  $|A_{0S}|$  components. From Figure 4.4 it becomes clear that expanding the space from II to III does not bring in anything new to splitting  $\Delta E$ . However, it will be unwise to jump at conclusion that the  $1p_{1/2}$  configuration is just ineffective. Instead, the expansion from space II to III should be analyzed in terms of behaviour of individual J levels with respect to the said expansion. In Figure 4.5 we have plotted the levels arising predominantly from  $(Of_{7/2})^2$

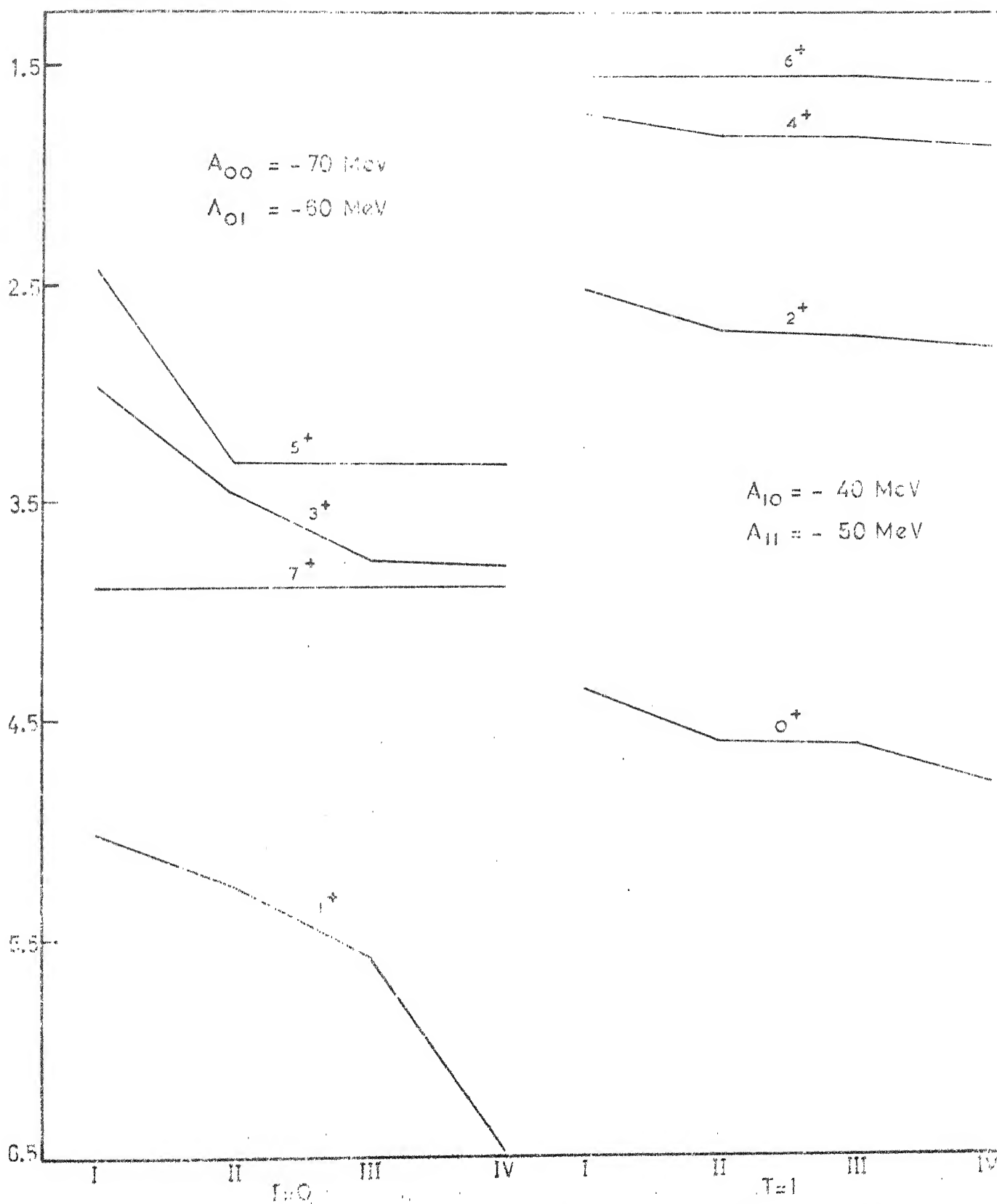


Fig. 4.5. Energy of levels arising predominately from  $(of_{7/2})^2$  configuration plotted as a function of space dimensionality (denoted by I, II, etc see the text)

configuration as calculated in the four spaces I, II, III and IV, including configuration mixing effects in the latter three for  $A_{00} = -70$  MeV,  $A_{01} = -60$  MeV,  $A_{10} = -40$  MeV and  $A_{11} = 50$  MeV. A study of Figure 4.5 clearly establishes that the effect on levels, of inclusion of the  $1p_{1/2}$  configuration in model space, is negligible and one might as well work without configurations  $(1p_{1/2} \text{ Of}_{7/2})$ ,  $(1p_{1/2} 1p_{3/2})$  and  $(1p_{1/2})^2$  for  $T = 1$  levels although it may not be said for  $(\text{Of}_{5/2} 1p_{1/2})$  configuration. Also, the effect of the  $1p_{1/2}$  configuration on  $1^+$  and  $3^+$  levels is substantial. Thus, at least few of the configurations may be ignored.

We make a relative study of curves for variation of  $|A_{1S}|$  strengths (Figures 4.3 and 4.4) at the two extremes of the range of values of  $|A_{1S}|$  parameters considered. We tabulate the corresponding values of  $\Delta E$  in Table 4.3. A relative study of the results, for difference between the values of  $\Delta E$  at the two extremities of the curves in different spaces, for the two spin components of the  $T = 1$  interaction shows that variation of  $A_{11}$  (odd  $\ell$ ) causes sharper change in  $\Delta E$  than does the  $A_{10}$  component (even  $\ell$ ). This is for  $(\text{Of}_{7/2})^2$  configuration (space I). However,

TABLE 4.3

In the first two columns the  $A_{1S}$  parameters are indicated. I, II etc. stand for space I, space II etc. In each of the spaces, the value of  $\Delta E$  corresponding to the particular  $A_{1S}$  set is shown. Within the same space, the change in value of  $\Delta E$ , as one goes from -40 MeV to -80 MeV for the particular spin component of the force, is also indicated.

$A_{10}$ (MeV)	$A_{11}$ (MeV)	Splitting $\Delta E$			
		I (MeV)	II (MeV)	III (MeV)	IV (MeV)
-70	-40	0.48	0.60	0.56	0.28
	-80	-0.47	-0.38	-0.36	-0.44
		} 0.95		} 0.92	
		} 0.98		} 0.72	
-40		0.30	0.50	0.55	0.60
-70					
-80		-0.39	-0.35	-0.37	-0.60
		} 0.69		} 0.92	
		} 0.85		} 1.20	

this difference in behaviour is reduced as the space expands, to the extent that in space IV,  $\Lambda_{10}$  causes sharper variation than does the  $\Lambda_{11}$  component meaning thereby that, effectively, in space IV even  $\ell$  states are dominant over odd  $\ell$  ones. This is also the general belief that contribution of even  $\ell$  states is stronger than that of odd  $\ell$  ones. Therefore, if we hold it, we can say that, for investigation of  $T = 1$  levels at least, one should adopt the full fp-shell as model space. Further, even in the space IV, although the even  $\ell$  states dominate over those of odd  $\ell$ , the contributions of the two types of  $\ell$  states are competitive so that unlike the case for  $T = 0$  interaction, it will not be justified to use a Serber force for  $T = 1$  spectroscopy.

For a given set of interaction parameters, energy levels plotted as a function of space dimensionality (Figure 4.5) clearly show that as the space is expanded from I to IV, at least the  $0^+$  and  $1^+$  levels continuously keep on moving down. Rather, for these levels the effect of including the  $0f_{5/2}$  configuration in model space is much more than that of including the  $1p_{1/2}$  configuration. It means that if an effective interaction is parametrized to fit the excitation spectra relative to ground state, we will end up with different parameters in different



spaces. This is, however, an established fact that phenomenological effective interactions are space dependent but the importance of the  $Of_{5/2}$  configuration puts a doubt over physical validity of parameters derived in space II or III. This is because we feel the effects of neglected configurations should be meaningfully absorbed in parameters only if these effects can be proved to be really small. Otherwise, as in the present problem, say for  $1^+$  level, we are seeing that the  $Of_{5/2}$  configuration is making a sharp effect on energy for a random set of parameters. An effective interaction can be derived in space III which might satisfactorily reproduce the  $1^+$  level but it can very well happen that if the  $1^+$  level position is calculated in space IV with same effective interaction parameters, the agreement would be lost. It only means that we may get the correct energy but not the correct wave function.

We have discussed the importance of  $Of_{5/2}$  level. We have seen that for  $1^+$  level, this configuration affects much more than any of other low-lying configurations. This further raises a doubt that similarly the effect of some still higher configuration might be too strong to be treated in effective interaction parameters. As such, it is appearing that whichever configurations contribute

strongly should be included directly in diagonalization so as to be explicitly included as a component in the wave function. It, therefore, becomes necessary to check the convergence of contributions of higher lying configurations as the space is expanded.

As mentioned earlier, we have not made exact diagonalization to consider the effect of configurations lying beyond  $fp$ -shell. However, then, we should first check as to how close is the approximation of replacing the correct diagonalized eigenvalue by the one calculated approximately through calculation of second-order contribution  $S$ . In Table 4.4 we list the second-order contributions of different configurations within  $fp$ -shell. All the second-order calculations have been done for

$$A_{00} = -70 \text{ MeV}$$

$$A_{01} = -40 \text{ MeV}$$

$$A_{10} = -40 \text{ MeV}$$

$$A_{11} = -50 \text{ MeV}$$

The approximate level energies obtained in this way are compared against those obtained by diagonalization in different spaces in Table 4.5. We see that approximation

TABLE 4.4

Results for calculation of second-order contributions of configurations above lowest  $(0f_{7/2})^2$  configuration, lying within fp-shell and contributing to  $0^+$  and  $1^+$  levels. These results are for  $A_{00} = -70$  MeV,  $A_{01} = -40$  MeV,  $A_{10} = -40$  MeV and  $A_{11} = -50$  MeV.

$J^\pi$	Excited configuration $ i_1 j_2\rangle$	Unperturbed excitation energy (MeV)	$\frac{\langle 0f_{7/2}^2   V   i_1 j_2 \rangle_J}{2}$ (MeV)	Second-order contribution (S) (MeV)
$0^+$	$(1p_{3/2})^2$	4	-1.1396	0.3247
	$(1p_{1/2})^2$	8	-0.5348	0.0357
	$(0f_{5/2})^2$	12.9	-1.1576	0.10385
$1^+$	$(1p_{3/2})^2$	4	-0.8230	0.1714
	$1p_{1/2} \ 1p_{3/2}$	6	-0.3444	0.01977
	$(1p_{1/2})^2$	8	0.2198	0.00604
	$0f_{5/2} \ 0f_{7/2}$	6.45	-0.9198	0.13117
	$0f_{5/2} \ 1p_{3/2}$	8.45	0.4382	0.02872
	$(0f_{5/2})^2$	12.9	-0.4124	0.013184

TABLE 4.5

Comparison of incorporation of effect of configuration mixing on  $0^+$  and  $1^+$  levels, arising predominantly from the  $(Of_{7/2})^2$  configuration, as calculated by exact diagonalization and by calculation of second-order contributions.

$J^\pi$	State	Energy in $(Of_{7/2})^2$ configuration (MeV)	Energy by exact diagonalization (MeV)	Approximately calculated energy (MeV)
$0^+$	II	-4.3576	-4.6014	-4.6823
	III		-4.6054	-4.7180
	IV		-4.7915	-4.8218
$1^+$	II	-4.1246	-4.2561	-4.2960
	III		-4.3501	-4.3218
	IV		-4.5804	-4.4839

works much better for  $1^+$  level where the predicted approximate energy falls above that obtained by diagonalization in both space III and IV. It means that if second-order effect of configurations beyond fp-shell can be shown to be substantial, it will mean that the effect of these configurations will be still more on diagonalization. However, for  $0^+$  level the second-order contribution overestimates the effect of mixing. Yet it does not mean that third-order contribution is important. For example, the second-order contribution of  $(1p_{3/2})^2$  configuration is 0.3247 MeV and the next correction is only 0.026 MeV (to be included with an opposite sign to that of the second-order contribution) which is really negligible and does not much account for the discrepancy between the  $0^+$  level energies in space II as obtained by diagonalization and by approximate calculation. Instead, the discrepancy might be attributed to underestimation of energy denominator which might be more than just the excitation energy of  $(1p_{3/2})^2$  configuration. The discrepancy is observed in all spaces. However, that can be seen to be because of the discrepancy in space II. Since the energy by diagonalization in space III is -4.6054 MeV and the second-order contribution of  $(0f_{5/2})^2$

and 0.13117 MeV respectively. Similarly, the contributions of  $(1p_{1/2})^2$  and  $(0f_{5/2} 1p_{3/2})$  configurations can be compared. Suppose we parametrize effective interaction in space III. Then we would be including all configurations upto  $(1p_{1/2})^2$  at 8 MeV without realizing that a configuration  $(0f_{5/2} 1p_{3/2})$  at 8.45 MeV is contributing about four times the 8 MeV configuration and is being excluded from model space just because the  $0f_{5/2}$  configuration is not being included in the model space. All the more, the  $(0f_{5/2} 0f_{7/2})$  configuration at 6.45 MeV contributes about 22 times the 8 MeV configuration and we are not including it for the similar reason. On the other hand, within space III, we are including the  $(1p_{1/2})^2$  configuration in diagonalization because it has been a convention to include all configurations including upto the highest  $j^2$  configuration without realizing that even within space III, the  $(1p_{1/2})^2$  configuration contributes much less than the leading contributor  $(1p_{3/2})^2$  configuration and once we are all out to determine an effective interaction only, it might as well be very good approximation to absorb so small effects in interaction parameters and drop this configuration at all from diagonalization. This puts a serious doubt on the way the model space

is arbitrarily chosen just by the consideration of single particle energy of an orbit and rest all are ignored just on the plea that they involve high single particle excitations. The contribution of  $(0f_{5/2})^2$  configuration to  $0^+$  level is 0.10385 MeV while that of  $(1p_{1/2})^2$  configuration is 0.0357 MeV. There is no reason to believe that contribution of, say,  $(0g_{9/2})^2$  configuration will not be comparable to that of  $(1p_{1/2})^2$  configuration at least. In Table 4.6 we present second-order contributions to levels other than  $0^+$  and  $1^+$ . The numbers vary over a wide range. Therefore, in Figure 4.6 we plot the logarithms of second-order contributions to different J levels versus the single particle excitation energy of the excited configuration. It is clear that the second-order contributions for all J levels vary erratically and single particle energy of a configuration can certainly not be the sole criterion for inclusion or exclusion of an excited configuration in model space. Even commonsense tells that instead of single particle energy of an orbit, the unperturbed energy of an excited two-particle configuration would be a more honest criterion for selection of model space. This can be seen even from the basic philosophy as to why do we have to include configuration mixing.

TABLE 4.6

Results for calculation of second-order contributions of configurations above lowest  $(0f_{7/2})^2$  configuration, lying within fp-shell and contributing to  $2^+$ ,  $4^+$ ,  $3^+$  and  $5^+$  levels respectively. These results are for  $A_{00} = -70$  MeV,  $A_{01} = -40$  MeV,  $A_{10} = -40$  MeV and  $A_{11} = -50$  MeV.

$J^\pi$	Excited Configuration $ j_1 j_2\rangle$	Unperturbed excitation energy (MeV)	$\frac{\langle 0f_{7/2}^2   V   j_1 j_2 \rangle_J}{2}$ (MeV)	Second-order contribution (S) (MeV)
1	2	3	4	5
$2^+$	$(1p_{3/2} 0f_{7/2})$	2	-0.5504	0.151470
	$(1p_{3/2})^2$	4	-0.4104	0.042106
	$(1p_{1/2} 1p_{3/2})$	6	0.2255	0.008474
	$(0f_{5/2} 0f_{7/2})$	6.45	-0.4251	0.028017
	$(0f_{5/2} 1p_{3/2})$	8.45	0.3010	0.010722
	$(0f_{5/2} 1p_{1/2})$	10.45	-0.3184	0.009701
	$(0f_{5/2})^2$	12.90	-0.0512	0.000203

Contd.



Contd. Table 4.6

1	2	3	4	5
$4^+$	$(1p_{3/2} \ 0f_{7/2})$	2	-0.4911	0.120580
	$(1p_{1/2} \ 0f_{7/2})$	4	0.1762	0.007761
	$(0f_{5/2} \ 0f_{7/2})$	6.45	-0.0261	0.000106
	$(0f_{5/2} \ 1p_{3/2})$	8.45	0.3009	0.010714
	$(0f_{5/2})^2$	12.90	-0.0598	0.000277
$3^+$	$(1p_{3/2} \ 0f_{7/2})$	2	-0.6781	0.229900
	$(1p_{3/2})^2$	4	-0.4089	0.041800
	$(1p_{1/2} \ 0f_{7/2})$	4	-0.3432	0.029445
	$(0f_{5/2} \ 0f_{7/2})$	6.45	-0.0723	0.000810
	$(0f_{5/2} \ 1p_{3/2})$	8.45	0.1444	0.002468
	$(0f_{5/2} \ 1p_{1/2})$	10.45	0.1296	0.001607
	$(0f_{5/2})^2$	12.90	-0.1515	0.001779
$5^+$	$(1p_{3/2} \ 0f_{7/2})$	2	-0.7547	0.284800
	$(0f_{5/2} \ 0f_{7/2})$	6.45	0.1044	0.001690
	$(0f_{5/2})^2$	12.9	0.0517	0.000207

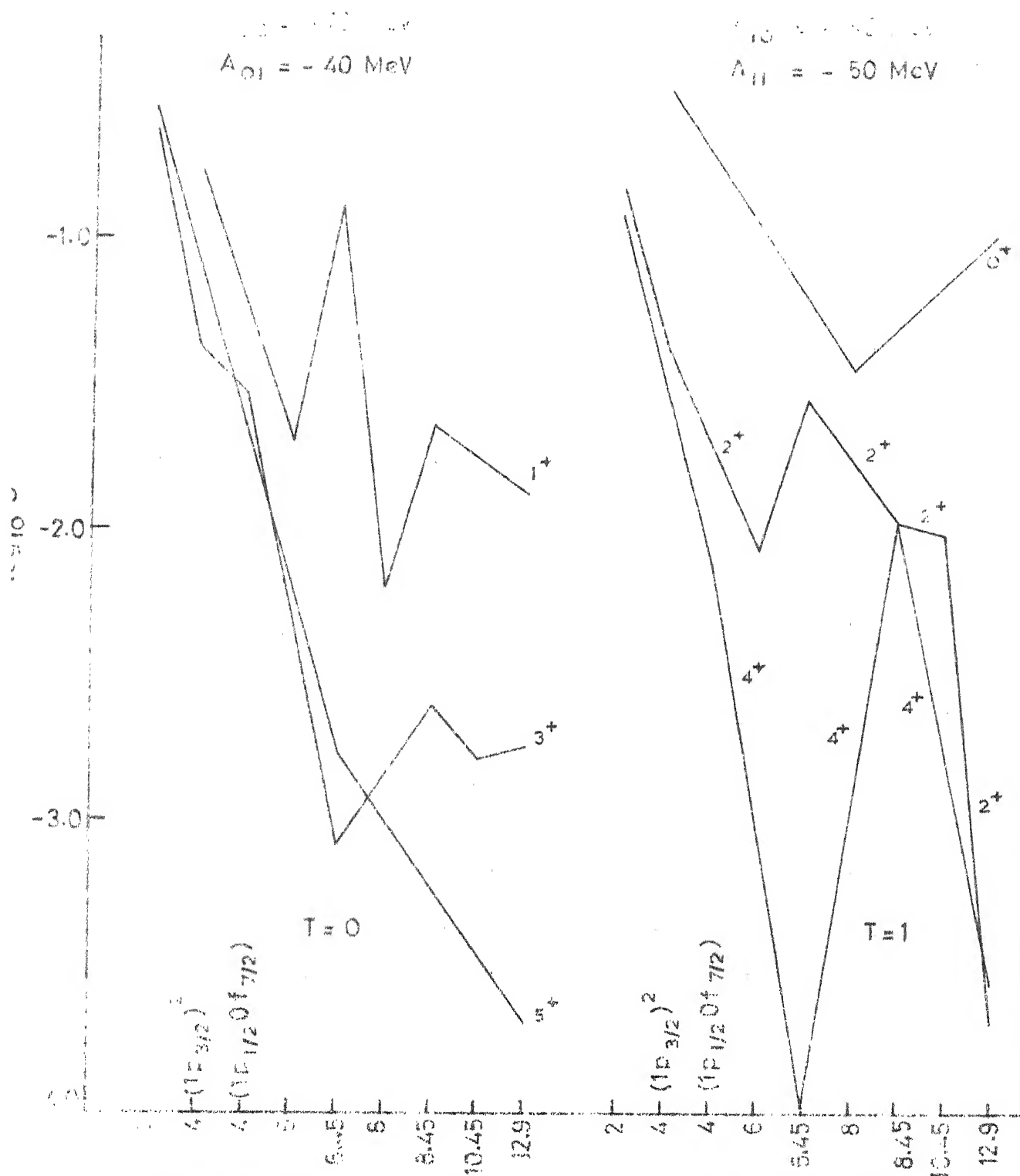


Fig. 4.6 Logarithm of second-order contributions (S) towards different J-levels arising from  $(1p_{7/2})^2$  configuration plotted as a function of the unperturbed excitation energy of the two-particle configuration (cf. table 4.6).  $J^\pi$  values are indicated on each graph.

In view of these doubts it becomes very necessary to see if saturation in respect of model space dimensionality is ever achievable. For this purpose we need to calculate the second-order contribution of configurations beyond fp-shell. However, correct single particle energies in this region are not established. Therefore, we adopt the level scheme as proposed by Mayer and Jensen<sup>146</sup> and arbitrarily assign single particle energies. These are shown in Table 4.7. As such, the numbers which we would arrive at should not be taken too literally. Yet this calculation is expected to give an approximate order-of-magnitude estimate of effect of high - lying configurations on low-lying levels. The results for  $0^+$  and  $1^+$  levels are tabulated in Tables 4.8 and 4.9 respectively. The logarithms of the numbers are plotted versus configuration number in Figures 4.7 and 4.8 respectively. It is very clear that the contributions keep on oscillating instead of monotonically decreasing as one hopes. We did not go beyond  $0i_{13/2}$  orbit but the trend of graphs makes it clear that convergence in level energies is not achieved upto 80 MeV configuration at least. Although no strict relationship could be established but, generally, for an excited  $|j_1 j_2 >$

TABLE 4.7

Single particle levels' sequence (taken from Mayer and Jensen<sup>146</sup>) used for calculation of second-order contributions from higher configurations. Except for first four configurations, single particle energies have been arbitrarily assigned.

S.No.	Orbit	Single Particle Energy (MeV)
1	0f <sub>7/2</sub>	0
2	1p <sub>3/2</sub>	2
3	1p <sub>1/2</sub>	4
4	0f <sub>5/2</sub>	6.45
5	0g <sub>9/2</sub>	9
6	0g <sub>7/2</sub>	15
7	1d <sub>5/2</sub>	17
8	1d <sub>3/2</sub>	19
9	2s <sub>1/2</sub>	21
10	0h <sub>11/2</sub>	23

Contd.

Contd. Table 4.7

S.No.	Orbit	Single Particle Energy (MeV)
11	$0h_{9/2}$	30
12	$1f_{7/2}$	32
13	$1f_{5/2}$	34
14	$2p_{3/2}$	36
15	$2p_{1/2}$	33
16	$0i_{13/2}$	40

TABLE 4.8

Results for Calculation of second-order contribution(5) of all configurations lying upto  $0i_{13/2}$  orbit contributing to  $0^+$  level arising from  $(0f_{7/2})^2$  configuration. Calculations have been done for  $A_{10} = -40$  MeV,  $A_{11} = -50$  MeV.

Configuration Index	Two-particle configuration $ j_1 j_2\rangle$	Unperturbed energy of the two-particle configuration (MeV)	$\langle 0f_{7/2}^2   V   i_1 j_2 \rangle_{0^+}$ (MeV)	Second-order contribution (5) (MeV)
1	2	3	4	5
1	$(1p_{3/2})^2$	4	-1.1396	0.3247
2	$(1p_{1/2})^2$	8	-0.5348	0.0357
3	$(0f_{5/2})^2$	12.9	-1.1576	0.10385
4	$(0g_{9/2})^2$	18	3.52341	0.68967
5	$(0g_{7/2})^2$	30	1.02577	0.035072
6	$(1f_{7/2} 0f_{7/2})$	32	-1.45856	0.06349
7	$(1d_{5/2})^2$	34	1.076165	0.034062
8	$(1d_{3/2})^2$	38	0.423915	0.0047289
9	$(2p_{3/2} 1p_{3/2})$	38	-0.230860	0.014026
10	$(1f_{5/2} 0f_{5/2})$	40.45	-0.182364	0.00082218

Contd.

Contd. Table 4.8

1	2	3	4	5
11	$(2s_{1/2})^2$	42	-0.289824	0.002
12	$(2p_{1/2} \ 1p_{1/2})$	42	-0.045978	0.000050334
13	$(0h_{11/2})^2$	46	-3.31757	0.23925
14	$(0h_{9/2})^2$	60	0.11258	0.00021123
15	$(1f_{7/2})^2$	64	-1.69937	0.045128
16	$(1f_{5/2})^2$	68	0.06972	0.000071481
17	$(2p_{3/2})^2$	72	-0.14019	0.00027295
18	$(2p_{1/2})^2$	76	-0.686875	0.0062078
19	$(0i_{13/2})^2$	80	1.594075	0.031765

TABLE 4.9

Results for calculation of second-order contribution (S) of all configurations lying upto  $0i_{13/2}$  orbit contributing to  $1^+$  level arising from  $(0f_{7/2})^2$  configuration. Calculations have been done for  $A_{00} = -70$  MeV,  $A_{01} = -40$  MeV.

Configu- ration Index	Two-particle configuration $ j_1 j_2\rangle$	Unperturbed energy of the two-par- ticle config- uration (MeV)	$\langle 0f_{7/2}^2   V   i_1 j_2 \rangle_{1^+}$ (MeV)	Second-order contribution (S) (MeV)
1	2	3	4	5
1	$(1p_{3/2})^2$	4	-0.8280	0.1714
2	$(1p_{1/2} 1p_{3/2})$	6	-0.3444	0.01977
3	$(0f_{5/2} 0f_{7/2})$	6.45	-0.9198	0.13117
4	$(1p_{1/2})^2$	8	0.2198	0.00604
5	$(0f_{5/2} 1p_{3/2})$	8.45	0.4382	0.02272
6	$(0f_{5/2})^2$	12.9	-0.4124	0.013184
7	$(0g_{9/2})^2$	18	3.28617	0.59994
8	$(0g_{7/2} 0g_{9/2})$	24	0.89231	0.033176
9	$(0g_{7/2})^2$	30	0.35501	0.0042011

Contd.



Contd. Table 4.9

1	2	3	4	5
10	(0h <sub>9/2</sub> 0f <sub>7/2</sub> )	30	-0.66186	0.014601
11	(1d <sub>5/2</sub> 0g <sub>7/2</sub> )	32	0.19106	0.0011407
12	(1f <sub>7/2</sub> 0f <sub>7/2</sub> )	32	-1.50360	0.070661
13	(1d <sub>5/2</sub> ) <sup>2</sup>	34	0.889495	0.023271
14	(1f <sub>5/2</sub> 0f <sub>7/2</sub> )	34	-0.112685	0.00037345
15	(1d <sub>3/2</sub> 1d <sub>5/2</sub> )	36	0.300596	0.0025099
16	(1f <sub>5/2</sub> 1p <sub>3/2</sub> )	36	-0.093983	0.00024536
17	(1d <sub>3/2</sub> ) <sup>2</sup>	38	0.035665	0.000033474
18	(2p <sub>3/2</sub> 1p <sub>3/2</sub> )	38	-0.214010	0.0012052
19	(1f <sub>7/2</sub> 0f <sub>5/2</sub> )	38.45	0.112685	0.00033022
20	(2s <sub>1/2</sub> 1d <sub>3/2</sub> )	40	0.180978	0.00081893
21	(2p <sub>3/2</sub> 1n <sub>1/2</sub> )	40	0.0091583	0.0000020969
22	(2p <sub>1/2</sub> 1p <sub>3/2</sub> )	40	-0.0091583	0.0000020969
23	(1f <sub>5/2</sub> 0f <sub>5/2</sub> )	40.45	-0.277804	0.001908
24	(2s <sub>1/2</sub> ) <sup>2</sup>	42	-0.189732	0.00085714
25	(2p <sub>1/2</sub> 1p <sub>1/2</sub> )	42	0.00299314	0.0000002133
26	(2p <sub>3/2</sub> 0f <sub>5/2</sub> )	42.45	-0.26451	0.0016482

Contd.

1	2	3	4	5
27	$(0h_{11/2})^2$	46	-3.700176	0.29762
28	$(0h_{9/2} \ 0h_{11/2})$	53	-0.470480	0.0041766
29	$(0h_{9/2})^2$	60	-1.543502	0.039709
30	$(1f_{7/2} \ 0h_{9/2})$	62	0.029784	0.000014309
31	$(1f_{7/2})^2$	64	-1.911334	0.057079
32	$(1f_{5/2} \ 1f_{7/2})$	66	-0.114136	0.00019739
33	$(1f_{5/2})^2$	68	-0.710628	0.0074264
34	$(2p_{3/2} \ 1f_{5/2})$	70	-0.264500	0.00099945
35	$(2p_{3/2})^2$	72	0.297558	0.0012297
36	$(2p_{1/2} \ 2p_{3/2})$	74	-0.566220	0.0043326
37	$(2p_{1/2})^2$	76	0.511348	0.0034404
38	$(0i_{13/2})^2$	80	1.399082	0.02447

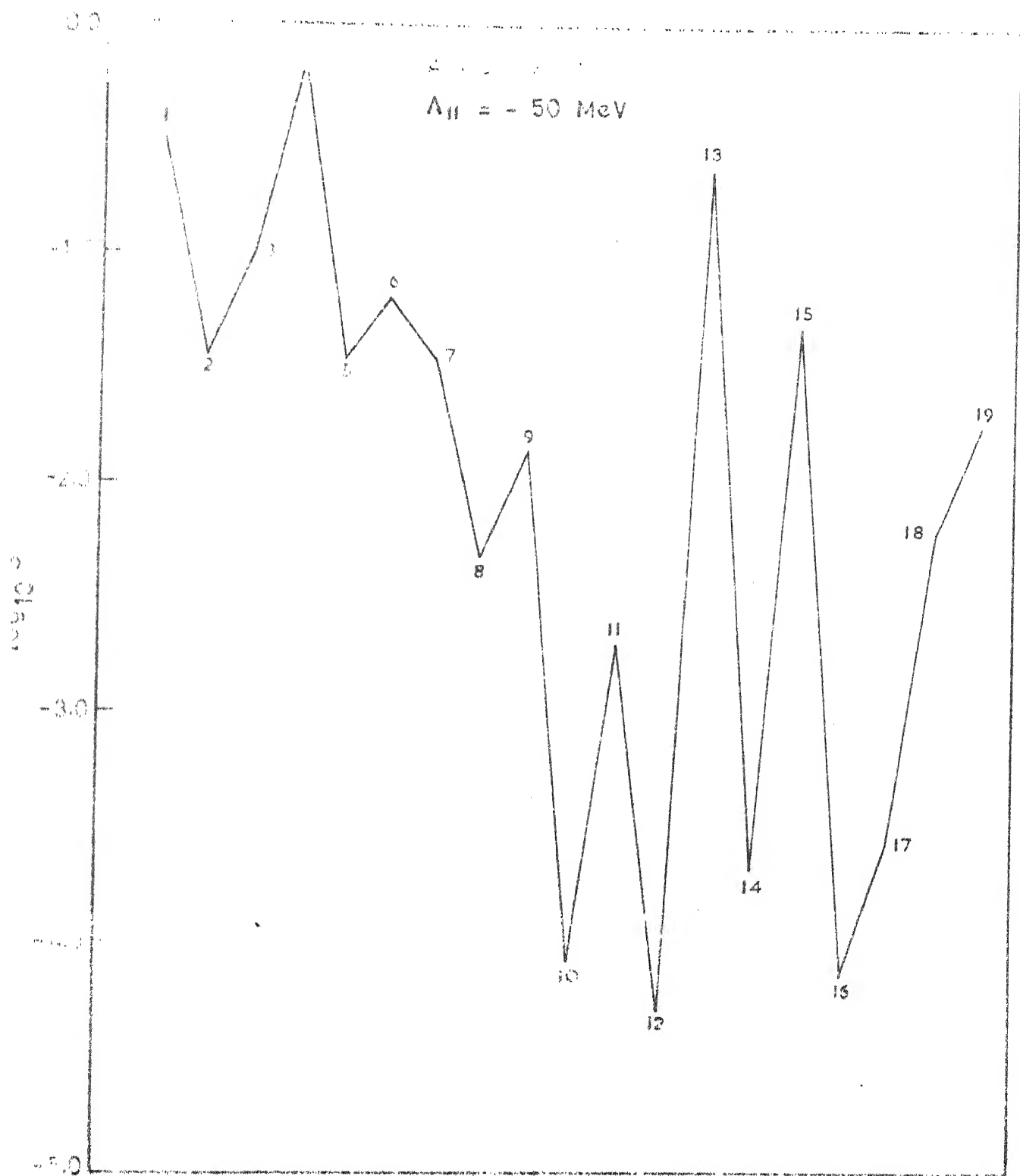


Fig 4.7. Logarithm of second-order contributions (S) towards  $0^+$  level arising from  $(\text{of } 7/2)^2$  configuration plotted as a function of index number of the excited two-particle configuration (Cf. table 4.8)

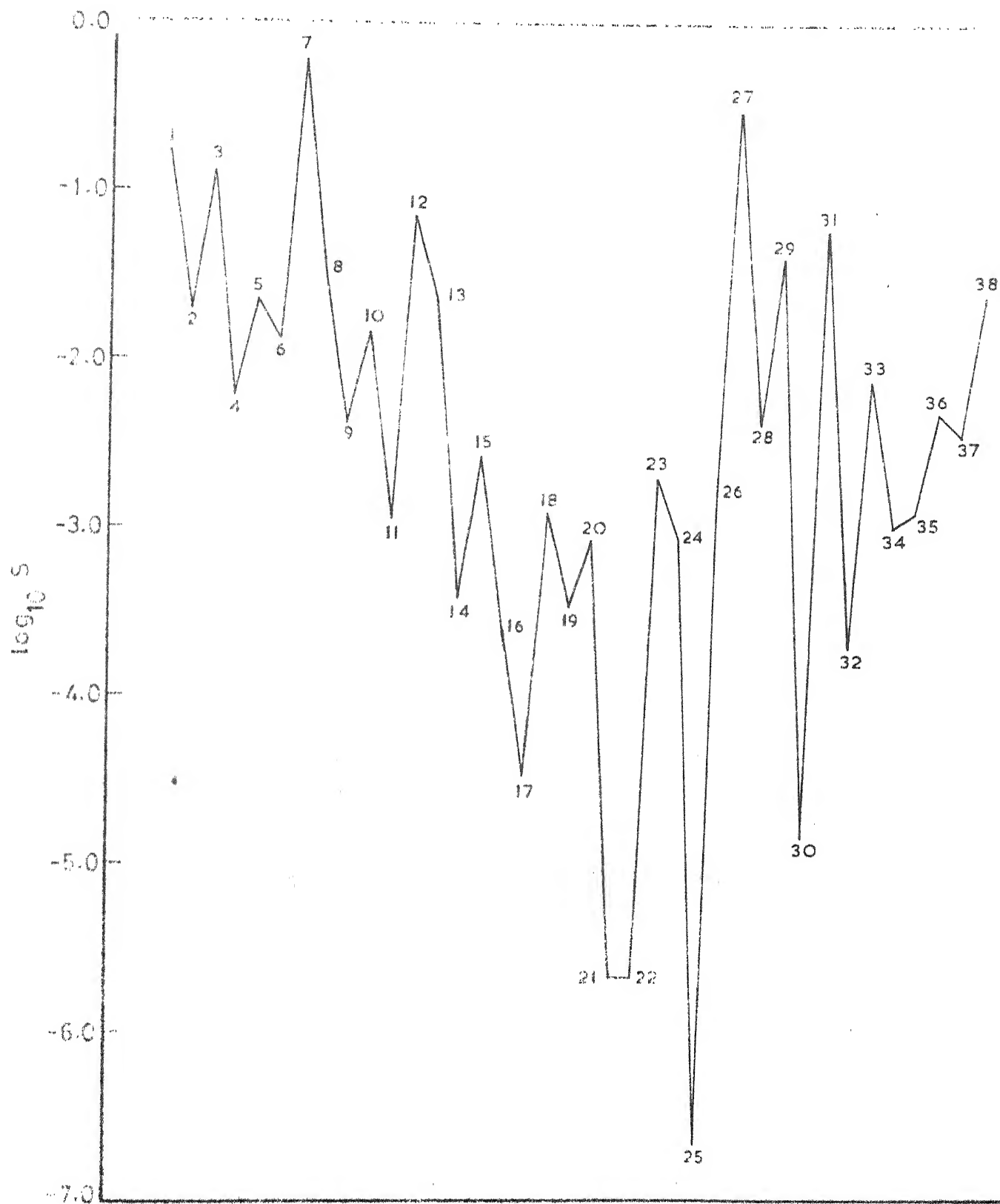


Fig. 4.8. Logarithm of second-order contributions ( $S$ ) towards  $1^+$  level arising from  $(\text{of } 7/2)^2$  configuration plotted as a function of index number of the excited two-particle configuration. (Cf. table 4.9)

configuration, the contribution is small for small  $j_1 + j_2$  like the 40 MeV and 42 MeV configurations for  $1^+$  level. Although contributions of both the 42 MeV configurations are negligible yet such a large difference - a factor of 4000 is not understandable on purely single particle 'energies' considerations. The contribution of the 30 MeV  $(0i_{13/2})^2$  configuration to  $1^+$  level is 0.02447 MeV and in view of practical limitations it can be neglected in comparison to 0.1714 MeV contribution of the 4 MeV configuration  $(1p_{3/2})^2$  but we should view it in comparison to the contribution 0.00604 MeV of the 8 MeV configuration  $(1p_{1/2})^2$  which we have always been including ! The contribution 0.59994 MeV of 18 MeV configuration  $(0g_{9/2})^2$  to  $1^+$  level is much more than any of the fn-shell configurations. We, therefore, argue that the  $(1p_{1/2})^2$  configuration can be neglected in favour of the  $(0i_{13/2})^2$  configuration and similarly the  $(0g_{9/2})^2$  and  $(0h_{11/2})^2$  configurations should also be explicitly included in diagonalization. We present some of such contrasting numbers in Table 4.10 for  $0^+$  level.

We have done these calculations for a randomly chosen set of parameters and for one nucleus and one

TABLE 4.10

Second-order contributions of some of the excited configurations contributing to  $0^+$  level arising from  $(0f_{7/2})^2$  configuration picked up so as to show that the unperturbed energy of the two-particle configuration cannot be the sole criterion for inclusion of a two-particle configuration in model space.

The excited state two-particle con- figuration	Unperturbed energy of the two-particle configuration (MeV)	Second-order contribution (s) (MeV)
$2s_{1/2}^2$	42	0.002
$2p_{1/2}^2$	42	0.000050334
$1d_{7/2}^2$	64	0.045128
$1d_{5/2}^2$	68	0.000071481
$2p_{1/2}^2$	76	0.0062078
$0i_{13/2}^2$	80	0.031765
$0f_{7/2}^2$	30	0.035072
$0i_{13/2}^2$	80	0.031765

might suspect if it is not going to be the case as faced by Cohen et.al.-merely an accident as proved later by Gupta and Trainor and by Engel and Unna. In the first place, even if such a thing happened on actual calculations in other shells, our results still stand where they are - that the nonconvergence may or may not come. Chances seem to be slim that such a thing would happen. Just to check, we calculated the effect of  $(Of_{7/2})^2$  configuration on  $0^+$  and  $1^+$  levels of  $(Od_{5/2})^2$  configuration and that of  $(Og_{9/2})^2$  configuration on  $0^+$  and  $1^+$  levels of  $(1p_{3/2})^2$  configuration. Same parameters as those used here were taken. The  $Of_{7/2}$  orbit was assumed 12 MeV above the  $Od_{5/2}$  orbit and the  $Og_{9/2}$  orbit was assumed to be 6 MeV above the  $1p_{3/2}$  orbit. The results are presented in Table 4.11. The results only substantiate our findings for the  $^{42}\text{Sc}$  nucleus. Choice of any other radial shape of the potential will certainly not make any drastic change in results. The strengths were also arbitrary and there is no reason why the general trend of results should not hold for other parameter values. Even the use of realistic interactions is not expected to make the things go the other way. Work of Joshi<sup>147</sup> has shown that realistic potentials can be satisfactorily simulated

TABLE 4.11

Second-order contributions of  $(Of_{7/2})^2$  and  $(Og_{9/2})^2$  configurations to  $(Od_{5/2})^2$  and  $(1p_{3/2})^2$  configurations for  $0^+$  and  $1^+$  levels. Calculations have been performed for  $A_{10} = -40$  MeV,  $A_{11} = -50$  MeV,  $A_{00} = -70$  MeV and  $A_{01} = -40$  MeV.

Matrix element (MeV)	Unperturbed energy of the two-particle configuration (MeV)	Second-order Contribution (S) (MeV)
$\langle Od_{5/2}^2   V   Of_{7/2}^2 \rangle_{0^+}$ = - 3.60574	24	0.54169
$\langle Od_{5/2}^2   V   Of_{7/2}^2 \rangle_{1^+}$ = -3.279268	24	0.448097
$\langle 1p_{3/2}^2   V   Of_{7/2}^2 \rangle_{0^+}$ = -1.37289	12	0.15708
$\langle 1p_{3/2}^2   V   Og_{9/2}^2 \rangle_{1^+}$ = 0.98742	12	0.08125



by phenomenological potentials and we can realize that in a study like the present one what matters is the parameters' values and not the way they have been derived - they may be phenomenological effective interaction derived to fit spectra or phenomenological potentials equivalent of realistic interactions. Conversely, the trend is also expected to hold if the realistic interaction itself is used.

#### IV.4 CONCLUSIONS:

Our study shows that a Serber type effective potential can be taken for  $T = 0$  interaction but not for  $T=1$  states. Further, it can be possible to roughly estimate beforehand that some of the configurations, which we might otherwise be going to include, really contribute very little and they can as well be dropped from calculation. Like this by making a preliminary investigation, we can get a physically more meaningful effective interaction by including an equal number of more important effects in place of those dropped even without adding to computational difficulties. Further, it is not legitimate to arbitrarily choose a

model space just on the basis of single particle energy of highest orbit in the model space. Instead, our calculations show that even a highly excited two-particle configuration can contribute more strongly than a comparatively much low excited one. However, many of the configurations in going upto the highest configuration also contribute very weakly so that they are better dropped.

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## APPENDIX A

Wave function of a single nucleon of mass  $m$ , moving in a harmonic oscillator potential, is given by

$$\Psi_{n\ell m}(\vec{r}) = \frac{R_{n\ell}(r)}{r} Y_{\ell m}(\theta, \phi) \quad (\text{A.1})$$

The normalized solution, corresponding to energy eigenvalue

$$E_{n\ell} = (2n + \ell + \frac{3}{2})\hbar\omega \quad (\text{A.2})$$

is given by

$$R_{n\ell}(r) = \sqrt{\frac{2^{1-n+2} (2\nu)^{\ell + \frac{3}{2}} (2\ell + 2n + 1)!!}{\sqrt{\pi} [(2\ell + 1)!!]^2 n!}} r^{\ell+1} e^{-\nu r^2} v_{n\ell}(2\nu r^2) \quad (\text{A.3})$$

where,

$$v_{n\ell}(x) = \sum_{k=0}^n (-)^k 2^k \binom{n}{k} \frac{(2\ell+1)!!}{(2\ell+2k+1)!!} x^k \quad (\text{A.4})$$

and

$$\nu = \frac{m\omega}{2\hbar} \quad (\text{A.5})$$

The wave function for two nucleons' relative motion is also given by above expressions provided  $\nu$  is

replaced by  $V' = \frac{\mu \omega}{2\hbar}$  where  $\mu$  is the reduced mass of the particles. For two nucleons,  $\mu = \frac{m}{2}$ . Hence,

$$R_{n\ell}(r) = \sqrt{\frac{2^{\ell-n+2} (V)^{\ell+\frac{3}{2}} (2\ell+2n+1)!!}{\sqrt{\pi} [(2\ell+1)!!]^2 n!}} r^{\ell+1} e^{-\frac{1}{2} V r^2} v_{n\ell}(V r^2) \quad (\text{A.6})$$

where  $V$  is same as defined above and  $r = |\vec{r}_1 - \vec{r}_2|$ .

A properly antisymmetrized and normalized two-particle wave function in  $jj$  - coupling is given by

$$\begin{aligned} |n_1 \ell_1 j_1, n_2 \ell_2 j_2 : JM, TM_T \rangle_{AS} \\ = N \left[ |n_1 \ell_1 j_1, n_2 \ell_2 j_2 : JM, TM_T \rangle \right. \\ \left. - (-)^{j_1+j_2+1+J+T} |n_2 \ell_2 j_2, n_1 \ell_1 j_1 : JM, TM_T \rangle \right] \end{aligned} \quad (\text{A.7})$$

where the convention is maintained that angular momentum of particle 1 is coupled to angular momentum of particle 2 (in this order) and  $N$  is given by

$$N = \frac{1}{(2+2 \delta_{n_1 n_2} \delta_{\ell_1 \ell_2} \delta_{j_1 j_2})^{1/2}} \quad (\text{A.8})$$

The expression for properly antisymmetrized and normalized matrix element of two-body interaction  $V$  between two such states is given by

$$\begin{aligned}
 & \langle n_1 \ell_1 j_1, n_2 \ell_2 j_2 : JT | V | n'_1 \ell'_1 j'_1, n'_2 \ell'_2 j'_2 : JT \rangle_{AS} \\
 &= 2^{NN'} \left[ \langle j_1, j_2 : JT | V | j'_1 j'_2 : JT \rangle \right. \\
 & \quad \left. + (-)^{j'_1 + j'_2 + J+T} \langle j_1, j_2 : JT | V | j'_2, j'_1 : JT \rangle \right]
 \end{aligned}
 \tag{A.9}$$

where other quantum numbers have been dropped.

The expression for matrix element can also be given in a form where matrix elements appearing on right side of eq. (A.9) are calculated in L S coupling

$$\begin{aligned}
 & 2^{NN'} \sum_{LS} A \begin{pmatrix} \ell_1 & \frac{1}{2} & j_1 \\ \ell_2 & \frac{1}{2} & j_2 \\ L & S & J \end{pmatrix} A \begin{pmatrix} \ell'_1 & \frac{1}{2} & j'_1 \\ \ell'_2 & \frac{1}{2} & j'_2 \\ J_1 & S & J \end{pmatrix} \times \\
 & \times \left[ \langle n_1 \ell_1, n_2 \ell_2 : LM_L | V | n'_1 \ell'_1, n'_2 \ell'_2 : LM_L \rangle \right. \\
 & \quad \left. - (-)^{\ell'_1 + \ell'_2 + L+S+T} \langle n_1 \ell_1, n_2 \ell_2 : LM_L | V | n'_2 \ell'_2, n'_1 \ell'_1 : LM_L \rangle \right]
 \end{aligned}
 \tag{A.10}$$



However, (A.10) holds strictly for central forces which conserve L and it is assumed that spin and isospin dependence of V has been calculated separately.

In the method of Slater integrals, the direct and exchange terms in eq. (A.10) are separately calculated using

$$\langle n_1 \ell_1, n_2 \ell_2; LM_L | V | n'_1 \ell'_1, n'_2 \ell'_2; LM_L \rangle = \sum_{k=0}^{\infty} F^k f_k \quad (\text{A.11})$$

where

$$f_k = (-1)^{\ell_1 + \ell'_1 + L} \sqrt{(2\ell_1+1)(2\ell_2+1)(2\ell'_1+1)(2\ell'_2+1)} \begin{pmatrix} \ell_1 & k & \ell'_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell_2 & k & \ell'_2 \\ 0 & 0 & 0 \end{pmatrix} \left\{ \begin{matrix} \ell_1 & \ell_2 & L \\ \ell'_2 & \ell'_1 & k \end{matrix} \right\} \quad (\text{A.12})$$

and

$$F^k = \int_0^{\infty} \int_0^{\infty} R_{n_1 \ell_1}(r_1) R_{n_2 \ell_2}(r_2) v_k(r_1, r_2) R_{n'_1 \ell'_1}(r_1) R_{n'_2 \ell'_2}(r_2) dr_1 dr_2 \quad (\text{A.13})$$

$$= \frac{2k+1}{2} \int_0^{\infty} \int_0^{\infty} \int_{-1}^1 R_{n_1 \ell_1}(r_1) R_{n_2 \ell_2}(r_2) V(|\vec{r}_1 - \vec{r}_2|) P_k(\cos \omega_{12}) R_{n'_1 \ell'_1}(r_1) R_{n'_2 \ell'_2}(r_2) dr_1 dr_2 d(\cos \omega_{12}) \quad (\text{A.14})$$

where,

$$\cos \omega_{12} = \frac{\vec{r}_1 \cdot \vec{r}_2}{r_1 r_2} \quad (\text{A.15})$$

Defining,

$$\begin{aligned} \vec{r} &= \vec{r}_1 - \vec{r}_2 \\ \vec{R} &= \frac{1}{2} (\vec{r}_1 + \vec{r}_2) \end{aligned} \quad (\text{A.16})$$

and

$$\cos \alpha = \frac{\vec{r} \cdot \vec{R}}{rR}$$

Hence,

$$\cos \omega_{12} = \frac{R^2 - \frac{1}{4} r^2}{r_1 r_2} \quad (\text{A.17})$$

The Legendre function  $P_k(\cos \omega_{12})$  can be expressed as a polynomial in  $\cos \omega_{12}$ . A volume element  $r_1^2 dr_1 r_2^2 dr_2 d(\cos \omega_{12})$  in  $(r_1, r_2, \omega_{12})$  representation becomes  $r^2 dr R^2 dR d(\cos \alpha)$  in  $(r, R, \alpha)$  representation. Hence, finally, the integrand in eq. (A.14) becomes a function of  $r, R$  and  $\alpha$ . Thus,

$$P^k = \frac{2k+1}{2} \int_0^\infty \int_0^\infty \int_{-1}^1 \frac{R_{n_1} \ell_1(r_1) R_{n_1'} \ell_1'(r_1)}{r_1^2} \cdot \frac{R_{n_2} \ell_2(r_2) R_{n_2'} \ell_2'(r_2)}{r_2^2} \cdot$$

$$V(r) P_k(\cos \omega_{12}) r^2 dr R^2 dR d(\cos \alpha) \quad (\text{A.18})$$

are calculated using the method of Slater integrals.

$$\langle n_1 \ell_1, n_2 \ell_2 : LM_L | V^Q | n'_1 \ell'_1, n'_2 \ell'_2 : LM_L \rangle = F^2 f_2 \quad (A.24)$$

where,  $f_2$  is calculated from (A.12) and the Slater integral  $F^2$  is calculated from (A.13)

$$F^2 = \int_0^\infty \int_0^\infty R_{n_1} \ell_1(r_1) R_{n_2} \ell_2(r_2) r_1^2 r_2^2 R_{n'_1} \ell'_1(r_1) R_{n'_2} \ell'_2(r_2) dr_1 dr_2 \quad (A.25)$$

They are tabulated in the appendix C. In eq. (A.23)

$\chi$  is the strength parameter.

Matrix elements of the spin-dependent  $\delta$ -function

force

$$V = v_0 \left[ 1 - \alpha + \alpha (\vec{\sigma}_1 \cdot \vec{\sigma}_2) \right] \delta(\vec{r}_1 - \vec{r}_2) \quad (A.26)$$

are given by

$${}_{AS} \langle n_1 \ell_1 j_1, n_2 \ell_2 j_2 : JT | V | n'_1 \ell'_1 j'_1, n'_2 \ell'_2 j'_2 : JT \rangle_{AS}$$

$$= \frac{NN'}{2\pi} [\ell_1] [\ell_2] [\ell'_1] [\ell'_2] \times$$

$$\times \left[ \int_0^\infty \frac{1}{r^2} R_{n_1} \ell_1(r) R_{n_2} \ell_2(r) R_{n'_1} \ell'_1(r) R_{n'_2} \ell'_2(r) dr \right] \times$$

Expression Contd. on next page

$$\begin{aligned}
& \sum_{\lambda S} V_{0S}^{\lambda} \begin{pmatrix} \ell_1 & \frac{1}{2} & j_1 \\ \ell_2 & \frac{1}{2} & j_2 \\ \lambda & S & J \end{pmatrix} \begin{pmatrix} \ell'_1 & \frac{1}{2} & j'_1 \\ \ell'_2 & \frac{1}{2} & j'_2 \\ \lambda & S & J \end{pmatrix} \\
& \begin{pmatrix} \ell_1 & \ell_2 & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell'_1 & \ell'_2 & \lambda \\ 0 & 0 & 0 \end{pmatrix} [1 - (-)^{S+T}]
\end{aligned}
\tag{A.27}$$

where, the notation  $[x] = \sqrt{x+1}$  and  $V_{0S}$  is strength in the particular spin-state  $S$ . For two identical nucleons  $T = 1$  and hence, via a  $\delta$ -function force, the antisymmetry condition requires that they can interact in spin singlet state only and the expression finally reduces to

$$\begin{aligned}
& (-)^{\ell_1+j_2+\ell'_1+j'_2+1} \frac{V_0}{2\pi} \times \\
& \times [\ell_1][\ell_2][\ell'_1][\ell'_2][j_1][j_2][j'_1][j'_2] \times \\
& \times \begin{Bmatrix} \ell_1 & j_1 & \frac{1}{2} \\ j_2 & \ell_2 & J \end{Bmatrix} \begin{Bmatrix} \ell'_1 & j'_1 & \frac{1}{2} \\ j'_2 & \ell'_2 & J \end{Bmatrix} \begin{pmatrix} \ell_1 & \ell_2 & J \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell'_1 & \ell'_2 & J \\ 0 & 0 & 0 \end{pmatrix} \\
& \times \left[ \int_0^\infty \frac{1}{r^2} R_{n_1} \ell_1(r) R_{n_2} \ell_2(r) R_{n'_1} \ell'_1(r) R_{n'_2} \ell'_2(r) dr \right]
\end{aligned}
\tag{A.28}$$

The radial integrals are tabulated in Appendix B.

In the method of Moshinsky brackets,

$$\begin{aligned}
 & {}_{AS} \langle n_1 \ell_1 j_1, n_2 \ell_2 j_2 : JT | V | n'_1 \ell'_1 j'_1, n'_2 \ell'_2 j'_2 : JT \rangle_{AS} \\
 &= 2 \sum_{\substack{\lambda S \lambda' \\ n \ell N \\ L n' J' \\ \ell'}} NN' (-)^{\lambda + \lambda'} \begin{pmatrix} \ell_1 & \frac{1}{2} & j_1 \\ \ell_2 & \frac{1}{2} & j_2 \\ \lambda & S & J \end{pmatrix} \begin{pmatrix} \ell'_1 & \frac{1}{2} & j'_1 \\ \ell'_2 & \frac{1}{2} & j'_2 \\ \lambda' & S & J \end{pmatrix} \times \\
 &\quad \times (2J'+1) [(2\lambda+1)(2\lambda'+1)]^{1/2} \\
 &\quad \times [1 - (-)^{\ell+S+T}] \begin{Bmatrix} n_1 \ell_1 & n_2 \ell_2 \\ n \ell & N L \end{Bmatrix} \begin{Bmatrix} n'_1 \ell'_1 & n'_2 \ell'_2 \\ n' \ell' & N L \end{Bmatrix} \begin{Bmatrix} L & \ell & \lambda \\ S & J & J' \end{Bmatrix} \\
 &\quad \times \begin{Bmatrix} L & \ell' & \lambda' \\ S & J & J' \end{Bmatrix} \langle (n \ell, S) J' | V | (n' \ell', S) J' \rangle \quad (A.29)
 \end{aligned}$$

For central forces it reduces to

$$\begin{aligned}
 & 2NN' \sum_{\substack{\lambda S \\ n \ell N \\ L n'}} \begin{pmatrix} \ell_1 & \frac{1}{2} & j_1 \\ \ell_2 & \frac{1}{2} & j_2 \\ \lambda & S & J \end{pmatrix} \begin{pmatrix} \ell'_1 & \frac{1}{2} & j'_1 \\ \ell'_2 & \frac{1}{2} & j'_2 \\ \lambda & S & J \end{pmatrix} \times \\
 &\quad \times [1 - (-)^{\ell+S+T}] \begin{Bmatrix} n_1 \ell_1 & n_2 \ell_2 \\ n \ell & N L \end{Bmatrix} \begin{Bmatrix} n'_1 \ell'_1 & n'_2 \ell'_2 \\ n' \ell' & N L \end{Bmatrix} \langle n \ell | V | n' \ell' \rangle \\
 &\quad (A.30)
 \end{aligned}$$

$$\langle n\ell | V | n'\ell' \rangle \equiv I_{n\ell, n'\ell'} = \sum_p B(n\ell, n'\ell', p) I_p \quad (\text{A.31})$$

$$\frac{1}{2} (\ell + \ell') \leq p \leq \frac{1}{2} (\ell + \ell') + n + n' \quad (\text{A.32})$$

The Talmi integral  $I_p$  is same as  $I_{Op}$

$$I_p \equiv I_{Op} = \int_0^\infty \frac{R_{Op}(r)}{r} V(r) \frac{R_{Op}(r)}{r} r^2 dr \quad (\text{A.33})$$

In general,

$$I_{n\ell, n'\ell'} = \int_0^\infty \frac{R_{n\ell}(r)}{r} V(r) \frac{R_{n'\ell'}(r)}{r} r^2 dr \quad (\text{A.34})$$

where the radial wave functions are for relative motion.

Thus, (A.33) reduces to

$$I_p = \frac{2^{p+2}}{\sqrt{\pi} (2p+1)!!} \int_0^\infty r^{2p+2} e^{-\gamma r^2} V(r) dr \quad (\text{A.35})$$

which is consistent with (A.19).

The radial integral  $I_{n\ell, n\ell}$  is also denoted by  $I_{n\ell}$ .

Matrix elements of the two-particle spin-orbit interaction

$$V_{LS} = V(r) \vec{\ell} \cdot \vec{S}$$

are given by

$$\begin{aligned}
 & {}_{AS} \langle n_1 \ell_1 j_1, n_2 \ell_2 j_2 : JT | V_{LS} | n'_1 \ell'_1 j'_1, n'_2 \ell'_2 j'_2 : JT \rangle_{AS} \\
 &= 2V_T (-)^{J+P} \sum_{\substack{\lambda \lambda' \\ n \ell \nu \\ l n'}} A \begin{pmatrix} \ell_1 & \frac{1}{2} & j_1 \\ \ell_2 & \frac{1}{2} & j_2 \\ \lambda & 1 & J \end{pmatrix} A \begin{pmatrix} \ell'_1 & \frac{1}{2} & j'_1 \\ \ell'_2 & \frac{1}{2} & j'_2 \\ \lambda' & 1 & J \end{pmatrix}^* \\
 & \times B \begin{matrix} n_1 \ell_1 & n_2 \ell_2 \\ n & \ell \end{matrix} \begin{matrix} n'_1 \ell'_1 & n'_2 \ell'_2 \\ n' & \ell \end{matrix} \begin{matrix} (\lambda) & (\lambda') \\ N & N \end{matrix} \begin{matrix} \ell & \ell' \\ L & L \end{matrix} [1 - (-)^{\ell+1+T}]^* \\
 & \times \sqrt{6 \ell (\ell+1) (2\ell+1) (2\lambda+1) (2\lambda'+1)} \times \\
 & \left\{ \begin{matrix} \lambda & \lambda' & 1 \\ 1 & 1 & J \end{matrix} \right\} \left\{ \begin{matrix} \lambda & \lambda' & 1 \\ \ell & \ell & L \end{matrix} \right\} I_{n \ell n' \ell} \quad (A.36)
 \end{aligned}$$

where  $P = 2n + \ell + 2N + L$

with the condition

$$\lambda' = \lambda, \lambda \pm 1 \quad (A.37)$$

Matrix elements of the tensor force

$$V_T = \left( \frac{32}{5} \pi \right)^{1/2} V(r) \vec{Y}_2(\theta, \phi) \cdot \vec{x}_2 \quad (A.38)$$

where  $\vec{Y}_2$  is the Racah tensor whose components are the spherical harmonics  $Y_{2m}(\theta, \phi)$  and  $\vec{X}_2$  is the rank two Racah tensor whose  $m = 0$  component is

$$X_{20} = \frac{1}{\sqrt{2}} (3 s_z^2 - s^2) \quad (\text{A.39})$$

are calculated from

$$\begin{aligned} & {}_{AS} \langle n_1 \ell_1 j_1, n_2 \ell_2 j_2 : JT | V_T | n'_1 \ell'_1 j'_1, n'_2 \ell'_2 j'_2 : JT \rangle_{AS} \\ &= 2NN' \sum_{\lambda \chi} \sum_{n \ell N} \sum_{n' \ell' N'} (-1)^{P+J+1+\ell} A \begin{pmatrix} \ell_1 & \frac{1}{2} & j_1 \\ \ell_2 & \frac{1}{2} & j_2 \\ \lambda & 1 & J \end{pmatrix} A \begin{pmatrix} \ell'_1 & \frac{1}{2} & j'_1 \\ \ell'_2 & \frac{1}{2} & j'_2 \\ \chi & 1 & J \end{pmatrix} \\ & \times \begin{matrix} n_1 \ell_1 & n_2 \ell_2 & n'_1 \ell'_1 & n'_2 \ell'_2 \\ \text{B} & (\lambda) & \text{B} & (\chi) \\ n & \ell & N & L \end{matrix} \times \\ & \times [1 - (-1)^{\ell+1+T}] \sqrt{120(2\lambda+1)(2\chi+1)(2\ell+1)(2\ell'+1)} \times \\ & \times \left\{ \begin{matrix} \lambda & \chi & 2 \\ 1 & 1 & J \end{matrix} \right\} \left\{ \begin{matrix} \lambda & \chi & 2 \\ \ell' & \ell & L \end{matrix} \right\} \begin{pmatrix} \ell & 2 & \ell' \\ 0 & 0 & 0 \end{pmatrix} I_{n \ell n' \ell'} \quad (\text{A.40}) \end{aligned}$$

with the condition

$$\begin{aligned} \chi &= \lambda, \lambda \pm 1, \lambda \pm 2 \\ \ell' &= \ell, \ell \pm 2 \end{aligned}$$



In the formalism of second quantization, confining to two-body interactions only, the Hamiltonian is defined by

$$H = \epsilon_0 + \sum_{\alpha\beta} C_{\alpha\beta} a_{\alpha}^{\dagger} a_{\beta} + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | V | \gamma\delta \rangle a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma} \quad (\text{A.41})$$

where  $\epsilon_0$  is some reference energy,  $C_{\alpha\beta}$  is the one-body part of the Hamiltonian - the kinetic energy,

$$C_{\alpha\beta} = \langle \alpha | t | \beta \rangle = \epsilon_{\alpha} \delta_{\alpha\beta} \quad (\text{A.42})$$

and  $\langle \alpha\beta | V | \gamma\delta \rangle$  are unantisymmetrized matrix elements of  $V$  taken between the two-particle states  $|\alpha\beta\rangle$  and  $|\gamma\delta\rangle$ .

Let us consider a closed shell nucleus whose ground state be denoted by  $|0\rangle$  such that all states below a sharply defined Fermi momentum are completely filled and those above completely empty. Then, relative to the ground state, the particle (p) and the hole (h) states are defined through

$$a_p |0\rangle = 0$$

$$a_h^{\dagger} |0\rangle = 0$$

where  $a$  and  $a^{\dagger}$  are respectively the particle annihilation and creation operators, the subscript collectively denotes the quantum number of state on which they act.

The creation of a hole state and a particle state is then defined by respectively,

$$|j_h m_h\rangle = (-)^{j_h - m_h} a_{j_h, -m_h} |0\rangle$$

$$|j_p m_p\rangle = a_{j_p m_p}^+ |0\rangle$$

The particle and hole states defined like this behave similarly under rotations, and hence can be coupled through C.G. coefficients, whereas the states  $a_{j_h m_h} |0\rangle$  and  $a_{j_p m_p}^+ |0\rangle$  do not. The somewhat different structure of the hole state creation operator from the corresponding particle state creation operator arises from the fact that relative to a ground state of total angular momentum zero, a hole state  $|j_h m_h\rangle$  will be created when a particle from the state  $|j_h - m_h\rangle$  is destroyed. Thus,

$$a_{j_h - m_h} |0\rangle = | (j_h - m_h)^{-1} \rangle$$

where the symbol  $'-1'$  signifies vacancy in the particular quantum state. In shell model description, an excited state in a closed shell nucleus occurs when a particle from the Fermi sea is lifted to one of the empty orbits. Therefore, a total angular momentum coupled hole-particle

excited state will be obtained as

$$|(j_h^{-1} j_p) JM\rangle = \sum_{m_h, m_p} (-)^{j_h - m_h} C_{m_h m_p}^{j_h j_p J} a_{j_p m_p}^+ a_{j_h - m_h} |0\rangle \quad (\text{A.43})$$

We make a term - by - term calculation of matrix elements of  $H$  between two such h-p states.

$$\langle j_h^{-1} j_p : JM | \epsilon_0 | j_h^{-1} j_p : JM \rangle = \epsilon_0 \delta_{j_p j_p'} \delta_{j_h j_h'} \quad (\text{A.44})$$

$$\langle j_h^{-1} j_p : JM | t | j_h^{-1} j_p : JM \rangle = \delta_{j_p j_p'} \delta_{j_h j_h'} (\epsilon_{j_p} - \epsilon_{j_h}) \quad (\text{A.45})$$

$$\langle j_h^{-1} j_p : JM | V | j_h^{-1} j_p : JM \rangle = - \sum_{\substack{m_h m_p m_h' \\ m_p' J' M'}} (-)^{j_h - m_h + j_h' - m_h'} C_{m_h m_p m_h'}^{j_h j_p J} C_{m_h m_p m_h'}^{j_h j_p J'} \langle j_h j_p : J' M' | V | j_h j_p : J' M' \rangle_{AS}$$

$$= - \sum_{J'} (2J'+1) \left\{ \begin{matrix} j_h j_p J \\ j_h j_p J' \end{matrix} \right\} \langle j_h j_p : J' M' | V | j_h j_p : J' M' \rangle_{AS} \quad (\text{A.46})$$

If isospin is also included

$$\begin{aligned}
 & \langle j_h^{-1} j_p : J^T | V | j_h^{-1} j_p : J^T \rangle \\
 &= - \sum_{J'T'} (2J'+1) (2T'+1) \left\{ \begin{matrix} j_h & j_p & J \\ j_h' & j_p' & J' \end{matrix} \right\} \\
 & \quad \left\{ \begin{matrix} \frac{1}{2} & \frac{1}{2} & T \\ \frac{1}{2} & \frac{1}{2} & T' \end{matrix} \right\} \langle j_h j_p : J'T' | V | j_h j_p : J'T' \rangle_{AS}
 \end{aligned}
 \tag{A.47}$$

In a detailed derivation where all the terms are retained on the right of eqs. (A.45), (A.46) and (A.47), there come terms which represent the core energy and the interaction of the hole and the particle with the core. The latter interactions can be ignored if one takes energies of single particle levels from experiment since experimental numbers absorb all effects to all orders. In a calculation where one needs to calculate the total binding energies of the levels, one also requires the core energy. However, in cases where one is required only to calculate the excitation energies of levels relative to the ground state, the core energy term simply drops out.

APPENDIX B

Tables of the integrals

$$\int_0^{\infty} \frac{1}{r^3} R_{n_1} \ell_1(r) R_{n_2} \ell_2(r) R_{n'_1} \ell'_1(r) R_{n'_2} \ell'_2(r) dr$$

let

$$I(n_1 \ell_1, n_2 \ell_2, n'_1 \ell'_1, n'_2 \ell'_2) \\ = \int_0^{\infty} \frac{1}{r^2} R_{n_1} \ell_1(r) R_{n_2} \ell_2(r) R_{n'_1} \ell'_1(r) R_{n'_2} \ell'_2(r) dr$$

The integrals are tabulated below in units of  $\frac{1}{\sqrt{2\pi}} \left( \frac{m\omega}{\hbar} \right)^{3/2}$

i) Op - shell:

$$I(01,01,01,01) = \frac{5}{6}$$

ii) 1s - 01 - shell

$$I(0s,0s,02,01) = \frac{1}{2^3} \cdot \frac{21}{5}$$

$$I(02,02,10,02) = - \frac{1}{2^3} \cdot \frac{7}{\sqrt{10}}$$

$$I(10,02,10,02) = \frac{1}{2^3} \cdot \frac{5}{2}$$

$$I(10,02,10,10) = - \frac{1}{2^3} \cdot \frac{3}{4} \sqrt{\frac{2}{5}}$$

$$I(10,10,10,10) = \frac{1}{2^3} \cdot \frac{41}{4}$$

iii) 3f-1p shell:

$$I(03,03,03,03) = \frac{429}{1120}$$

$$I(03,03,03,11) = -\frac{1}{2^5} \cdot \frac{99}{10} \sqrt{\frac{2}{7}}$$

$$I(03,03,11,11) = \frac{1}{2^5} \cdot \frac{69}{10}$$

$$I(03,11,11,11) = -\frac{1}{2^5} \cdot \frac{17}{60} \sqrt{14}$$

$$I(11,11,11,11) = \frac{1}{2^5} \cdot \frac{121}{100}$$

iv) 2s - 1d - 0g shell:

$$I(12,12,12,12) = \frac{1}{2^{10}} \cdot \frac{13158}{35}$$

$$I(12,12,20,12) = -\frac{1}{2^{10}} \cdot \frac{517}{735} \sqrt{\frac{7}{15}}$$

$$I(12,12,04,12) = -\frac{1}{2^{10}} \cdot \frac{110}{7} \sqrt{2}$$

$$I(12,12,20,20) = \frac{1}{2^{10}} \cdot \frac{2419}{10}$$

$$I(20,20,20,20) = \frac{1}{2^{10}} \cdot \frac{8257}{8}$$

$$I(12, 12, 04, 20) = \frac{1}{2^{10}} \frac{706}{\sqrt{350}}$$

$$I(12, 12, 04, 04) = \frac{1}{2^{10}} \cdot \frac{17732}{105}$$

$$I(20, 12, 20, 20) = - \frac{1}{2^{10}} \frac{435}{4\sqrt{7}}$$

$$I(04, 04, 04, 04) = \frac{1}{2^{10}} \frac{3087}{10}$$

$$I(20, 12, 04, 20) = - \frac{1}{2^{10}} \cdot 39$$

$$I(20, 12, 04, 04) = - \frac{1}{2^{10}} \frac{1166}{3\sqrt{7}}$$

$$I(20, 20, 04, 20) = \frac{1}{2^{10}} \frac{137}{4} \sqrt{\frac{2}{7}}$$

$$I(20, 20, 04, 04) = \frac{1}{2^{10}} \cdot \frac{445}{3}$$

$$I(04, 12, 04, 04) = - \frac{1}{2^{10}} \frac{572\sqrt{2}}{7}$$

$$I(04, 20, 04, 04) = \frac{1}{2^{10}} \frac{286}{3} \sqrt{\frac{2}{7}}$$

All other integrals needed in any of the above mentioned major shells and not written here explicitly, can be shown to be equal to one of those mentioned, e.g.

$$I(20,12,20,12) = I(12,12,20,20)$$



APPENDIX C

Tables of Slater integrals for the quadrupole force:

i) Op-shell:

$$F^2(\text{Op}, \text{Op}, \text{Op}, \text{Op}) = \frac{25}{16 \nu^2}$$

ii) 1s-Od shell:

$$F^2(\text{Od}, \text{Od}, \text{Od}, \text{Od}) = \frac{49}{16 \nu^2}$$

$$F^2(\text{Od}, \text{Od}, 1s, \text{Od}) = - \frac{35}{8 \nu^2} \sqrt{\frac{2}{5}}$$

$$F^2(\text{Od}, \text{Od}, 1s, 1s) = \frac{5}{2 \nu^2}$$

$$F^2(1s, \text{Od}, \text{Od}, 1s) = \frac{5}{2 \nu^2}$$

iii) Of - 1p shell:

$$F^2(\text{Of}, \text{Of}, \text{Of}, \text{Of}) = \frac{81}{16 \nu^2}$$

$$F^2(\text{Of}, \text{Of}, \text{Of}, 1p) = - \frac{63}{8 \nu^2} \sqrt{\frac{2}{7}}$$

$$F^2(0f, 0f, 1p, 1p) = \frac{7}{2 \mathcal{V}^2}$$

$$F^2(0f, 1p, 0f, 1p) = \frac{81}{16 \mathcal{V}^2}$$

$$F^2(0f, 1p, 1p, 0f) = \frac{7}{2 \mathcal{V}^2}$$

$$F^2(0f, 1p, 1p, 1p) = -\frac{63}{8 \mathcal{V}^2} \cdot \sqrt{\frac{2}{7}}$$

$$F^2(1p, 1p, 1p, 1p) = \frac{81}{16 \mathcal{V}^2}$$

iv) 2s - 1d - 0g shell:

$$F^2(1d, 1d, 1d, 1d) = \frac{121}{16 \mathcal{V}^2}$$

$$F^2(1d, 0g, 1d, 0g) = \frac{121}{16 \mathcal{V}^2}$$

$$F^2(0g, 0g, 0g, 0g) = \frac{121}{16 \mathcal{V}^2}$$

$$F^2(1d, 1d, 1d, 2s) = -\frac{11\sqrt{7}}{4 \mathcal{V}^2}$$

$$F^2(1d, 1d, 1d, 0g) = - \frac{33\sqrt{2}}{8 \nu^2}$$

$$F^2(1d, 1d, 2s, 2s) = - \frac{7}{\nu^2}$$

$$F^2(1d, 1d, 2s, 0g) = - \frac{3\sqrt{14}}{2 \nu^2}$$

$$F^2(1d, 1d, 0g, 0g) = - \frac{9}{2 \nu^2}$$

$$F^2(1d, 0g, 2s, 0g) = - \frac{11\sqrt{7}}{4 \nu^2}$$

$$F^2(1d, 0g, 0g, 0g) = - \frac{33\sqrt{2}}{8 \nu^2}$$